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CALCULATION OF THE GLASS TRANSITION TEMPERATURES OF LINEAR POLYMERS PART 3 EVALUATION OF CALCULATION RELATIONSHIPS

by.

W.A. Lee

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CALCULATION OF THE GLASS TRANSITION TEMPERATURES OF LINEAR POLYMERS
PART 3 EVALUATION OF CALCULATION RELATIONSHIPS

bу

W. A. Lee

SUMMARY

Four equations, relating the structure of polymers in numerical form to their glass transition temperatures (Tg)s, are evaluated using a large data set of 1179 polymers. Additive temperature parameters, for the relationship giving the best fit to the data, are tabulated which enable predictions to be made of many polymer Tgs outside the data set. These parameters also provide a measure of the relative effectiveness of groups in internally plasticising polymers.

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This is Part 3 of a series of Reports on the calculation of the glass transition temperatures (Tgs) of linear polymers. An earlier Technical Memorandum emphasised the importance and significance of the Tg¹, Part ! of this series described how a large data set of polymers could be ordered unambiguously², and Part 2 described the data set itself³.

Since the glass transition temperature (Tg) of polymers was first observed, workers have attempted to relate polymer chemical structures to their Tgs and interest in the subject is reflected in the fact that there have been over 100 papers on the calculation of Tgs since 1965. Unfortunately, the polymer data sets to which the relationships have been applied have been insufficiently large, in most cases, to provide an adequate test of their validity; the data chosen could have provided, adventitiously a better fit to the relationships than might be found with a different, or larger, polymer data set. The significance of the size of, and distribution of polymers and groups within, the present data set of 1179 polymers has been discussed³.

In the present Report, the results of applying four relationships to the 1179 polymer data set are described. Additive temperature parameters (ATPs) are calculated which may be used in the prediction of polymer Tgs; these parameters also provide a measure of the relative effectiveness of groups in internally plasticising polymers. This Report goes on to provide analytical data on the results in the form of tables which facilitate updating of the data set by correlating calculation errors with specific polymers and groups. However, this aspect is not pursued in discussion as the main object of this Report is to provide the already-mentioned ATPs.

2 RELATIONSHIPS EVALUATED

Some of the relationships evaluated have been used before on a small data set of polymers having alkyl side chains 4. A much larger set of such polymers are included in the present data set. The previous analysis did not use the Bayesian statistics of the present calculation and therefore did not provide ATPs for each chemical group as does the treatment described here 5,6. There are other distinctions. The relationships tested in the present analysis are:

$$Tg = \sum_{\ell=1}^{\ell=x} (n_{\underline{i}} Tg_{\underline{i}})$$
 (1)

$$\frac{1}{Tg} = \sum_{i=1}^{k=x} \left(\frac{w_i}{Tg_i} \right), \qquad (2)$$

 $\frac{1}{Tg} = \sum_{i=1}^{i=x} \left(\frac{n_i}{Tg_i} \right) , \qquad (3)$

and

$$lnTg = \sum_{i=1}^{i=x} (n_i lnTg_i) , \qquad (4)$$

where Tg = glass transition temperature of the polymer,

Tg; = the additive temperature parameter (ATP) of the ith group,

n; = mole fraction of the ith group,

w. = weight fraction of the ith group

and x = the number of groups in the polymer.

In this treatment, a 'group' is considered to be the smallest polymer segment capable of independent torsional oscillation with respect to its nearest neighbours and is otherwise as previously defined3. Each group is identified by an arbitrary code number and the nearest neighbours are considered to be invariant. Dependant as the Tg is on the barriers to rotation between groups and their nearest neighbours, this condition is considered to be an essential aspect of the present treatment. Equation (1) has been successfully applied previously 7,8 to smaller data sets in a different type of statistical analysis. This equation would be the same as the simplified form of the DiMarzio and Gibbs relationship if n; represented the fraction of rotatable (flexible) bonds in the ith group and Tg; were equal to, or a constant fraction of, the T2 value of a homopolymer of the ith group; T, is the temperature below which such a polymer possesses zero configurational entropy. However, the application of the equation here is purely empirical and embodies the assumption that the Tg of a polymer is a linear function of the Tg contributions of its constituent groups in proportion to their mole fractions, with the important qualification, repeated for emphasis, that the neighbours of the single-groups are invariable 2,3

The application of the first equation is illustrated with respect to the first polymer of Table 5 of Part 2 3 whose structure, in numerical terms is reproduced below. * indicates the beginning of a new polymer data line, so "833 1" is a continuation line.

The polymer, identified as number 1, contains eight groups, has a Tg of 219 K, has one each of groups type 56, 57, 58, 59, 60 and 833, and two groups of type 72.

$$219 = (56 + 57 + 58 + 59 + 60 + 72 + 72 + 833)/8$$

where the group numbers, within parentheses, are here used to identify the parameter numbers of groups, (ATPs or Tg_is), not the parameter values. Thus, for example, 56 is a parameter number for group 56 which has a value whose units are in degrees K. The Tg is therefore seen to be equated to the average Tg_i (or ATP).

The statistical treatment of the equations is described elsewhere 5,6.

3 RESULTS

Each of the equations provided a set of ATPs for the groups in the data set. From these parameters the Tgs of all the polymers were calculated and Table ! shows the rms of the difference between calculated and observed Tgs (rms) for the four equations.

Table 1

Equation	rms (K)
1	12.6
2	15.6
3	21.1
· 4	15.2

Evidently, the first equation provides the lowest rms error. The maximum error in calculated Tg (see below) is associated with the same polymer, polymer 1325, for all equations. This polymer has a side-chain of 10 carbon atoms next to a heterocyclic ring and the published Tg may have been accorded to disordering of the carbon chain and be a sub-transition, rather than Tg which is normally regarded as marking substantial rotational liberation in the main chain. However, data have not been excluded from the set unless it was more certain that either the structure of the polymer, or the Tg value were positively in doubt. If the errors in calculated Tg are compared with the polymer structures it will be found that in many instances the higher Tg errors are associated with polymers having long carbon-chain sequences. Table 2 (microfiche) provides details on the difference (DIFF) between observed and estimated Tgs for each polymer using the different equations. In the table, DIFF, FDIFF, HDIFF and LDIFF relate to equations (1) to (4), respectively.

As the lowest errors are associated with equation (1), and equations (1), (3) and (4) are much easier to apply than equation (2), which requires a group

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weight parameter, the remainder of this discussion of results is restricted to those deriving from the use of equation (1).

A major interest of the present work stems from the need to know the relative contributions of different groups to the Tgs of polymers. Table 3 therefore shows the ATPs associated with each group in numerical order of increasing ATP and Table 4 presents the same data, but in hierarchical order 2 of the main (or central) single-group and simultaneously in increasing numerical order of ATP in respect of groups having the same main single-group, but one, or more, different neighbours; main- (M) and side-chain groups (S) are differentiated. This differentiation applies to the central group only. Though it is not the purpose of this Report to do other than present the results in the tables, it will be noted that numerous comparisons may be made between structures and ATPs. In general, despite the empirical nature of the relationships, it is seen that those factors which hinder rotation of the main group with respect to the neighbouring groups, such as polar interaction, bulkiness, steric factors, etc, tend to raise the ATP, and conversely, as is well known for polymer Tgs.

A disturbing feature of the results, despite the low rms error, is the large error in calculated Tg (>20 K) associated with 121 out of 1179 polymers. An analysis is therefore presented showing which polymers are associated with particular calculated Tg errors, Table 5 (microfiche computer printout), and which groups are associated with particular calculated Tg errors, Table 6 (microfiche computer printout). In Table 6, the columns are from left to right: line number (line 1 is not represented), group number, average Tg error (TGE), maximum Tg error, and paired numbers representing polymer number and associated Tg error for however many polymers contained the particular group. Continuation lines are distinguished by having no entries in the second to the fourth columns.

4 CONCLUSIONS

Of four equations, relating the structure of polymers in numerical form to their glass transition temperatures (Tg)s, the best fit, to a large data set of 1179 polymers, is provided by the equation relating the Tg to the mole fraction of groups in the polymers expressed in terms of group additive temperature parameters. An important proviso of the treatment is that the nearest neighbours of groups should be invariant.

Additive temperature parameters, for the relationship giving the best fit to the data, are tabulated which enable predictions to be made of many polymer Tgs outside the data set. These parameters also provide a measure of the relative effectiveness of groups in internally plasticising polymers.

-N=-N=-N=-N=N=	-\$1-0-\$1-	-CH ₂ -NHCH ₂ -	CF ₂
162 (M) ATP -72	874 (M) ATP -S2	519(M) ATP 0	773(S) ATP 44
NH-E-	\$ CH ₂ CH ₂	-с-о-сн-	-0CHCHZ- CH2
561 (N) ATP 52	741 (S) RTP 54	1000 (M) ATP 58	572 (N) ATP 67
	-S-NH-	NH-C-	-N=P-
591(S) ATP 68	1962(N) ATP 69	1963 (M) ATP 69	625(S) ATP ^T 70
-CH-		-ç+sc+ _z -	-\$:- CH ₂ CH ₃
548(\$) ATP 90	1165(N) ATP 99	546(M) RTP 115	924(S) ATP 115
-CF ₂ CF ₂ CF ₂ -	-N=	-cH=CH—CHZ-CHZ CIS	0 CH ₂ CH ₂
165 (M) ATP 123	163(S) ATP 126	122 (M) ATP 127	59(S) ATP 129
-0 ⁻ 2-5-0 ⁻ 2-	-P0CH ₂ -	-CHZ-CHZ-CHZ-	ĊΗ ₂ CΗ— CΗ ₂ -
643 (M) ATP 131	975 (M) ATP 132	13(M) ATP 133	236(S) ATP 138
CH- CH ₂ CH ₂ S57(S) ATP 138	CH ₂ 68(S) ATP 139	-C 0 CF ₃ 49(S) ATP 140	-\$n- CH ₂ CH ₂ 814(S) ATP 147
-CH=CH-CH2-CH2-TRANS	CH3 -NHSINH- CH3	-CH- C=0 P	-N= - NM CH ₂
123(M) ATP 149	508(M) ATP 151	57(S) ATP 153	818(S) ATP 153

1 K 0004

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-сн ₂ -{ сн ₂ }-, сн ₂ -	СН ₃ -СН ₂ —\$1—СН ₂ - СН ₃	-ċ Сн ₂ Сн ₃
1321 (M) ATP 155	588(M) ATP 157	841(S) ATP 158
CH ₂ CF ₂ 181(S) ATP 159	CH ₂ CH ₂ CF ₃ 421(S) ATP 159	CI -N= -N= -N= - 0 441(M) ATP 160
-0	CH ₃ -SI-CH ₃ 951 (S) ATP 163	CH ₂ CH ₂ CH ₂ CH ₂ 60(5) ATP 164
-s-s-cH ₂	-C=CHCH ₂ -CH ₂ - TRANS	NN NH-
538(M) ATP 165	849(M) ATP 166	1969(M) ATP 168
	-ŅСсн ₂ -	-N=PF ₂ N=PF ₂ -
1970(M) ATP 168	704(M) ATP 169	770(M) ATP 169
-cH2-{ CH2}2-CH2-	-осн ₂ çн	-cH=cHcHCH ₂ - cis cH ₃
1302 (M) ATP 169	645(M) ATP 170	372(M) ATP 171
С́Н2 [С́Н2] ₄ С́Н ₂	-сн ₂ -осн ₂ -	Сн ₂ [Сн ₂] ₂ Сн ₂
1354(S) ATP 172	99(M) ATP 174	1352(S) ATP 175

CH ₂ [CH ₂] ₅ CH ₂ 1355(S) ATP 175	CH2 [CH2]6 CH2 1356(S) ATP 175
2058 (M) ATP 175	-ÇF0CF ₂
N0CF ₂ 982 (N) ATP 177	N
CH ₃ -0-\$1-CH ₂	-çнсн ₂ сн ₂ -
-0CH ₂	-QCF ₂ CF ₂ -
797 (N) ATP 183 CH ₂ [CH ₂] ₃ CH ₂	-CH ₂ -CHCH ₂ -
1353(S) ATP 184 -N- CH ₃ -S ₁ -CH ₃ CH ₃	459 (M) ATP 185 -S-CF ₂ -S-
G12(S1 ATP 185 -CH- 0 CH ₂ 471(S) ATP 189	751 (M) RTP 185 0 C=0 726(S) RTP 191

			 _
о -с-о-сн ₂ -	-CH2 [CH2] CH2	-0CHCH ₂ - CH ₃	сн ³ -сн ⁵ -ссн ⁵ -
103 (M) ATP 193	1314(M) ATP 194	435(M) ATP 195	4(N) ATP 196
-sснсн ₂ - Сн ₂	[H ₂ [CH ₂] ₇ CH ₂	[-сн ₂ -{сн ₂ }-сн ₂ -
547 (M) ATP 197	1357(S) ATP 198	1359(S)_ATP 199	1305 (M) ATP 201
-cF _Z -{cF _Z } ₃ -cF _Z -	-CH− CH2	-ocNH	CH ₃ -CH ₂ -C=CH-CH ₂ CIS
1403 (M) ATP 201	235(S) ATP 202	445(M) RTP 202	304(M) ATP 203
-c=cнсн ₂ -сн ₂ - cis		-CH _Z -{ CH ₂ }-CH _Z -	CL -N=N=N=
891 (M) ATP 203	1452(S) ATP 203	1303 (M) ATP 204	637 (M) ATP 205
сн ₂ сн-	-NHNH-	C-CH _Z	-CH ₂ -{CH ₂ }-CH ₂ -
230(S) ATP 207	574(M) ATP 207	586(S) ATP 207	1307 (M) ATP 208
-0\$;0- CH3		-N=P- NCH ₂ - CH ₂	-сн _д sсн _д -
223 (M) RTP 209	796 (M) ATP 209	821(S) ATP 209	295(M) ATP 210
ξης [<mark>ςης</mark>] ¹⁰ ζης	-ch- 0 -cf ₃	-осн ₂ о-	-0—СН0- СН ₃
1360(S) ATP 210	164(S) ATP 213	425(M) RTP 213	455 (N) ATP 213
-cF ₂ -{cF ₂ }-cF ₂ -	-0CFCF ₂ - CF ₃		-s- -s -
1402(N) ATP 213	39(M) ATP 214	578(M) RTP 214	579(M) ATP 214

	-	,	
-сн ₂ -{ сн ₂ }-сн ₂ -	SYNDIOTACTIC -CH ₂ -CHCH ₂ - CH CH ₂	-oCÇH	-0s-
1304(M) ATP 215	531 (M) ATP 216	177 (M) ATP 218	1112(M) ATP 218
	CF ₂ [CF ₂] ₅ CF ₂	CH ₃ -\$1-CH ₃	СН ₃ —СН ₃
1456(S) ATP 219	1455(S) RTP 221	915(S) ATP 223	929(S) ATP 223
-CF- 0 CF ₃	CH ₂ S CH ₂	CH ₃ -CB ₅ H ₅ C510- CH ₃	-CH ₂ -{CH ₂ }-CH ₂ -
48(S) RTP 224	742(5) RTP 225	676(M) RTP 226	1308(M) RTP 226
-сн ₂ -{ сн ₂ }-сн ₂ -	о -ссн ₂ -сн-	N	-CH ₂ CF ₂ CH ₂
1309(M) ATP 226	291 (M) ATP 227	2212(S) ATP 227	494(M) RTP 228
-0NH-	-çнсн ₂ çн-	다 ₂ [다 ₂] B	CH ₃ -0-51CH ₂ - CH ₂
1237(M) ATP 229	833 (M) ATP 230	1358(S) ATP 230	467(M) ATP 231
-SCH ₂ S-	—N— - - - - - - - - - - - - - - - - - -	а -a—с—сн ₂ -	Сн—сн _з
543(M) ATP 231	1241(S) ATP 231	178(M) ATP 232	237(S) ATP 232
-CF ₂ { CF ₂ }CF ₂ -	;=0 0 0 1 7H2	-осн ₂ сн ₂ -	-0-CH ₂ -
1406(M) ATP 232	58(S) ATP 233	98(M) ATP 234	651(M) ATP 234

		
-s-c+-c- c+ ₃	-0NCF ₂ - CF ₂	
1910(M) ATP 235	981(M) ATP 237	2184(N) ATP 237
5-5-0	-\\!-\\	
2201 (M) ATP 237	3(M) ATP 236	454 (M) ATP 239
-sснсн ₂ - сн ₃	С1 -СH ₂ -ССH ₂ - С1	-N-21-N-
184(M) RTP 240	492(M) ATP 240	608 (M) ATP 240
ίн₂ [[н₂], , [н₂	-a5 <u>-</u> [a5 <u>]*a5</u> -	-\$1—CH _Z -\$1-
1361 (S) RTP 240	1404 (M) ATP 240	589(M) RTP 241
1361(S) RTP 240 -N=	-осн ₂ ¢	645 645 5-
647(5) RTP 241	846(M) RTP 241	864 (S) ATP 241
он- он ₂ он ₃	-sсн ₂ ¢	-Œ _Z -Œ½-Œ _Z -
105(S) ATP 242	555(M) ATP 242	493 (M) ATP 244
-¢носн ₂ -	CH2 [CH2]13	CH ₃ -0CCH ₂ - CH ₃
707 (M) ATP 244	1363(S) ATP 244	231 (M) ATP 246
-CF ₂ 0CF ₂ -	-ss	ÇF2 ÇF2 C1
452(M) ATP 246	545(M) RTP 248	609 (S) ATP 247

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-05 ₂ -0-0H ₂ -	ÇH₂	-CH ₂ -SI-CH ₂	-сн ₂ снсн ₂ -
159(H) RTP 248	731 (S) ATP 249	759(M) RTP 249 CH ₃	74 (M) RTP 251
ĊH− CH2 CH−		-CH ₂ -SICH ₂ -	CH2
334(S) ATP 252	525 (M) ATP 252	603(M) ATP 252	750(S) ATP 253
- ү - сн₂-сн₂-	-cf ₂ cfcf ₂ - 0	-cac-	-N==-
1106 (M) ATP 253	55(M) ATP 254	90 (M) ATP 254	636(S) ATP 254
-0СFСН ₂ - СF ₃	-ccH _Z CH _Z -	0 0 0 0 0 0	
2055 (M) RTP 255	14(M) ATP 256	259(S) ATP 256	785 (S) ATP 256
CH=CH- CH2 CH2 1164(N) ATP 256	F ₂ [F ₂] F ₂ 1454(9) ATP 256	443(S) ATP 257	-CH- CH ₂ CH ₃ SS4(S) ATP 257
0 -0CCF ₂ -	0 -CCF ₂ CF ₂ -	CH-CH ₃	S CH2 CH3
596 (M) ATP 257	597 (M) ATP 257 CH3 -0-51-0-	290(S) ATP 258 Br -N=P-N=P-N=P-	754(S) RTP 258
1400 (M) ATP 258	266(M) ATP 259	824(M) ATP 259	1312(M) ATP 260
CF ₂ CH ₂	-0-51-CH ₃	-N-C-N+-	CF ₂ CF ₂ NO ₂
183(S) ATP 263	710(M) ATP 265	1920 (M) ATP 265	29(S) ATP 266

			,
-cu2-cis cis	-CH- 9 CH3	Ç42	-0-04 <u>F</u>
120 (M) ATP 266	1048 (5) ATP 266	53(S) ATP 267	1301 (M) ATP 267
-CH ₂ -CFCH ₂ -	CH ₃ -CH ₂ -C=CH-CH ₂ -TRANS	다. 다. 다. 다.	-0-\$1-CH ₃
84 (M) ATP 268	307 (M) ATP 268	549(S) ATP 270	25 (M) ATP 271
	-00-	-cH=CH-	ليدي [إيدي ^ع] ¹⁴
979(S) ATP 271	988 (N) ATP 271	1166(M) ATP 271	1364(S) ATP 271
о Сн ₂ Сн ₃	- рн сн- сн ₂ -	-0-51 F	-СН- 0 1
64(S) ATP 272	385 (M) ATP 272	460 (M) ATP 273	497(S) RTP 274
\$=0 T'2 Ct'3 1053(S) ATP 274	-SCH ₂ CH ₂ - 102(H) ATP 275	-CH _Z -CH _Z -CH _Z -CH ₃ 658 (M) ATP 275	153(5) ATF 276
1000107 HTT 274	102(1) 111 213	000 (II) HII 210	
; <u>−</u> 0 ;+2	;≕0 ;н—сн ₃ ;н ₃	-CH2-CH=CH-CH2 TRANS	-CF ₂
653(S) ATP 276	1043(S) RTP 276	121 (M) ATP 277	594(M) ATP 277
CH ₂ N-CH ₂ CH ₂ 694(S) ATP 278	CF2 CF2 CF2 166(S) ATP 279	-CH ₂ CHCH ₂	CH—CH ₃ CF ₃ 624(S) ATP 280
037(3) NIF 2/0	100 (3) MIL 713	TOLVID HILL COV	957131 NII 699
-	olo		CF2-CF2
1763(M) ATP 280	1764 (M) ATP 280	1785(H) ATP 280	592 (M) ATP 281

			·
CF ₂ CF ₂	-\$1- CH ₂ CH ₂	-0NCF ₂ - CF ₃	-N- CF ₂ CF ₃
90 (S) ATP 282	884(S) ATP 282	33 (H) ATP 284	45(S) ATP 284
ф сн—сн _э сн _э	-\$1- -\$1-	D13	CH ₃
239(S) ATP 284	925(S) RTP 284	606(S) ATP 285	716(S) ATP 285
ςμ ₂ [ςμ ₂] ₁₅		-cH=CH-CH ₂ -CH- CIS	-cHCH=CHCH ₂ -
1365(S) ATP 285	129 (M) ATP 287	375(M) ATP 288	377(N) ATP 266
-012-01-012 01 012	CF-0-	-ar ₂	5-2 5-2 5-7-2 5-7-2
403(H) ATP 289	529 (N) ATP 289	847(N) ATP 289	790(S) ATP 290
-0-{ <u>-</u> 0+	073	Ç1-2 CF−	5+ 5-45 = 0
115(M) ATP 291	442(S) RTP 291	584(S) ATP 291	1138(S) ATP 291
		-¢-	-ar ² ar ² -br ² br ²
1774(M) ATP 291	826(S) RTP 292	933(S) ATP 292	382(N) ATP 293
CH2	-0-CH-CH ₂		-NHCH ₂
422(S) ATP 293	436(M) ATP 293	483 (NI ATP 293	1232 (M) ATP 293
сн ₃	-cr ₂ { cr ₂ }- ₈ -cr ₂ -		-\$1 <i></i> 04 ₂ -04 ₂ -
700(S) ATP 295	1408 (M) ATP 295	1574 (S) ATP 295	468 (M) ATP 296

and the same of

	 		
7 ² 7 ² 7 ₃	CH2 N-CH3	-0-CH2	-sсн ₂ рн-
768(S) ATP 296	1070(SI ATP 296	43(M) ATP 297	551 (N) ATP 297
-ç- CH ₂	000	N CF2-3-	
848(S) ATP 297	1531 (MI ATP 297	526 (M) ATP 298	1925(M) ATP 298
-C	-CH2-CHCH2 C=0	-5+c=-5+- p	- ç-6-ç -
1926(H) ATP 296	55 (H) RTP 299	132 (M) ATP 299	134(N) ATF 299
-ç- GH2 GH2	-CF ₂ CF ₂ CH ₂ -		-CH2-N N-CH2
810(S) ATP 299	10(H) ATP 300	1941 (M) ATP 300	1942(M) ATP 300
042 042	сн ₃ сн ₃ - с—сн ₃		-C-N
72(5) ATP 301	619(S) ATP 301	693(S) ATP 301	706(N) ATP 301
-CH2-N-CH2	CI 		-CH ₂ -{ CH ₂ }-CH ₂ -
1991 (M) RTP 301	139 (M) ATP 303	778(S) ATP 303	1306(M) ATP 303
CH3	-cr ₂ [cr ₂] ₅ -cr ₂ -		-cr ₂
819(S) ATP 304	1405(M) ATP 304	190(S) ATP 305	595(N) ATP 305
CH2 S CH3	5-15 5-15 5-14	-CH=CH CIS CH=CH CIS 0=C C=0	CIS
752(5) ATP 305	985(\$) RTP 305	1162 (M) ATP 305	1163 (M) ATP 305

			
-N= - NH CH ₃	62 [62] ² 62	-s-ay-l-	-¢¢
1170(S) ATP 305	1457 (S) ATP 305	583 (H) ATP 306	809(N) ATP 306
Ct√2 Ct√2 \$==0	6.00 Co.		-CHZ CHZ
1051(S) RTP 306	639(S) ATP 307	1770(M) RTP 307	44 (M) RTP 308
-\$1CFg-	CF ₃	-cf- 	- с нсғ _г -сн-
131 (N) ATP 308	179(S) ATP 308	88(S) ATP 309	135(M) ATP 309
-cr ₂ -c+-cr ₂ -	-64664-	-0-a ⁵ -a-	SYNDIOTACTIC
138(M) ATP 309	930 (H) RTP 309	36(M) ATP 310	535(H) ATP 310
CI	Z-Ct3	€ 013 013	-cNCH ₂ -
621(S) ATP 310	1046(S) ATP 310	646 (M) ATP 311	899(M) ATP 311
cr3 cr2 cr2	C=0 CH ₂	ال 12 ال 12 ارد	-0-CH2-
772(S) ATP 311	1135(S) ATP 311	1366(S) ATP 311	46(M) ATP 313
다. 다.—다.3 다.		o o o	0 CF—CF ₃ CF ₃
229(S) ATP 313	2158(M) ATP 315	793(S) ATP 317	191(S) ATP 318
72 73	-CH- -C2 -C3	CH ₃ -0-31-0- CH ₂	-CH2-SnCH2- CH2
778(S) ATP 318	194(5) ATP 319	283(M) ATF 319	780(\$) ATP 319

-\$ 0 	0 -C-s- p +-	-sc¢+-	-\$1NH\$1-	CH3
802(S) ATP 319	1909 (M) RTP 320	1911 (M) ATP 320	602(M) ATP 321	89(M) ATP 323
2-7-2 2-7-2 2-7-2	о п -с-сн-с- -ч ₂	-CH2	F 0-CH _Z	-0-F
1052(S) ATP 323	176(M) ATP 324	1233 (N) RTP 324	141(M) ATP 325	144(M) RTP 325
F 10-012	CH ₃ CB ₅ H ₅ CS10- 	-oC		\$ 50 -53
816(M) ATP 325	888 (M) ATP 325	92 (M) ATP 326	383(S) ATP 326	542 (S) ATP 326
-סיז-סיז-	- E-2	CH ₃ -CB ₁₀ H ₁₀ C\$10- METH CH ₃	сн ³	C1-C-C1 C1
656 (M) ATP 327	1034(S) ATP 327	1143 (M) ATP 327	328(S) ATP 328	581 (S) ATP 328
+-52	-pp	-N-C-0-	-€- \ -\-	0-013
709(S) ATP 328	138(M) ATP 329	1004(M) ATP 329	1790(M) ATP 329	311(S) ATP 330
CF2 CF2 Gr	The CH2	-0CH ₂ CF	-0CF ₂ CH ₂ -	
509(S) ATP 330	1866 (M) ATP 330	2054 (M) ATP 330	203 (M) ATP 331	507(S) ATP 331

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-\$1CH ₂ -\$	DH3	-\$1CF ₂ -	CH2 -0\$10- CH2
1015(H) ATP 331	1173(S) ATP 332	127(H) ATP 333	521 (M) RTP 333
-¢r- 9 \$F2	ÇF2 0 	С 0-сн ₃	-N- CF ₂ CF ₂
140(S) RTP 334	256(S) ATP 334	1032(S) ATP 334	28(S) ATP 33S
Ċ+2 C+3 Ç=0	-CH2-CHCH2-	Снсн ₂ -	-N=
638(S) ATP 335	1047(N) RTP 335	332(5) ATP 336	439(S) ATP 336
-CHz-CHCHz- CF3		-CH ₂ CH ₂ -CH ₂ -	-cf ₂ ccf ₂ -
715(H) ATP 336	1611(M) ATP 336	655 (M) ATP 337	50 (M) ATF 339
-ç 'cr₂- ç		O-CH2-0-	-{CH2}-CH2-0
51 (M) ATP 339	1059(S) RTP 339	674 (M) ATP 340	692 (M) RTP 340
-cH- CH3-CCH3 CH3	-CH2-CH2	0-	
2042(S) RTP 340	540(M) ATP 341	640(S) RTP 341	1723(H) ATP 341

-C- -C- -C- -C-		-Сн-сн ₂ -	-0-CF ₂ -
2032(S) RTP 341	300(5) ATP 342	649(H) ATP 342	800 (N) RTP 342
PH ₂	CH-CH ₃	Ct	-N-CH ^Z -CH ^Z
832(S) RTP 343	1022(\$) ATP 343	1082(S) ATP 343	1876 (H) ATP 343
	CH2 CF2	F2 53	-0-0-0-
2016 (H) ATP 343	470 (S) ATP 344	477(5) ATP 344	1263 (H) RTP 344
	- ç F ç F Cı	-91-	0 CH2-0-
1453(S) ATP 344	169 (M) ATP 345	905(M) ATP 345	669 (M) ATP 348
~-E-	Erz Erz		
1008 (H) ATP 346	1037(S) ATP 348	2011 (M) ATP 346	2113(H) ATP 348
-oco-	ç=0 CH—C≀ C≀	-C-N	-C
110(M) ATP 347	1045(3) RTP 347	1240(M) ATF 347	1017(M) ATP 348

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Ċ=0 CH2 Cl	-CH ₂	-\$1\$1- -\$1-
338(S) ATP 349	539(M) ATP 350	810(M) ATP 350
-t 0 CH ₃ 1073(S) ATP 350	CH ₃ -CH ₂ -CCH ₂ - 0 1074(M) ATP 350	1215 (M) ATP 350
10/3/3/ 1/1/ 330	(1874(1) 111 330	- 12.13 (II) AII 330
- CH3		C=0 CH2
2179(M) ATP 350	128(M) ATP 352	303(S) ATP 352
-N=P-		NH -N=P-N=P-N=P- NH
629(S) ATP 352	712(M) ATP 352	822 (M) ATP 352
-Ç0CH ₂ - 877 (M) ATP 352	1520(M) 978 352	CH ₃ -0-51-0- F 462 (M) ATP 353
677 (H) HIT 332	1620(M) ATP 352	462 (H) HIF 353
-CH=CH	← CH=CH-←	СН ₂ 0 СН ₃
1168 (M) ATP 353	1169(M) ATP 353	61 (S) RTP 354
FCH CF ₂ CH ₂	CH ₂ CH ₃	−\$1- - -C8 ₅ H ₅ C\$1-
777 (S) ATP 354	2030(S) RTP 354	675 (M) ATP 355

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	-осн ₂	ин Сн—сн ₃	- Ēr-Ēr-Ēr-
1738(M) ATP 355	1900 (M) ATP 355	405 (S) RTP 356	761 (M) RTP 356
CH2-CH2	-NH	-C-N-C-	
871 (M) ATP 356	1761 (M) ATP 356	1956 (M) RTP 356	801 (H) ATP 357
-NH - C - NH -	-N-NH-C-		CF ₂
1954(N) ATP 357	1955 (M) ATP 357	795 (M) ATP 358	253(S) ATP 359
C1.5	-cr ₂ -cr ₂ -		—α²–α²–
265 (S) RTP 359	791 (N) RTP 359	1029(S) ATP 359	1050(M) ATP 359
-CH ² -CH ² -H	-012-10-012-		C=0 0 0 0
1213(M) RTP 358	1211(M) ATP 360	1710(M) ATP 360	190(5) ATP 362
-NH-CH ₂	CH2 CH2 CH2	CH ₂ CH ₃ 993(S) ATP 362	-ICH2
523 (M) ATP 362	683 (S) ATP 362	227(2) HIL 207	1944(M) RTP 362
- c H-	-¢сн ₂ сн-	ç=0 Ç ^F 2 Ç ^F 2	─ -\$ -
614(S) ATP 363	627 (M) RTP 363	1142(S) ATP 363	1724(N) ATP 363
-0CH2			-scH ₂ -
1204(M) ATP 364	605 (S) ATP 365	686 (S) ATP 365	559(M) ATP 366

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		-N-E-CH2
1035(S) ATP 366	1111(M) ATP 366	1917(M) ATP 366
-CF ₂ CH ₂ CH ₂ -	CH3	-N-CH2-CH2
469 (M) RTP 367	1065(S) ATP 367	1993(M) ATP 367
CH3 -CB ₁₀ H ₁₀ C - 51CB ₁₀ H ₁₀ C - META CH3 META	-oc	- -
2013(N) ATP 367	599 (M) ATP 368	299(S) ATP 369
الله الله الله الله الله الله الله الله	—N— C=0 CH-	
1031(S) ATP 369	1136(S) ATP 369	2145(M) ATP 370
-0-10- C1	-ÇF	-c+2-c+-c+2
1812(M) ATP 371	528(H) ATP 372	107 (M) ATP 373
с <u>—</u> о	0-CH ₂	сн ₃ -с—сн ₃
457(S) RTP 373	541 (M) ATP 373	1021(S) ATP 373
¢=0 cι−c−cι cι	- ин сн ₂ сн ₂ -	CH3 -0-91-0-
1044(S) ATP 373	12(M) ATP 374	734 (H) RTP 374
	~opo N-	-01- C1 ₂ C1
746(S) RTP 374	994 (M) ATP 374	575(S) ATP 376

			
CH3		-o ₂ -o ₂ -	-CF- C=0 CH ₃
1036(S) ATP 376	1762 (M) ATP 376	157(H) RTP 377	732(S) ATP 377
○ G ₃		-N=N=	0- C=0 C+-
827 (M) ATP 377	1054(S) ATP 377	644 (M) RTP 378	2051(S) ATP 379
-cc+c-	-CF ₂ CFCF ₂ - Cl	-CH ₂ F CH ₂	- - - - - -
784 (H) RTP 380	137 (M) ATP 381	690(M) ATP 361	1049(S) ATP 381
المالية المالي	-5-0-5- N	CH=CH- CH=CH-	-\$1\$1-
688 (S) ATP 382	718(S) ATP 382	1167(M) ATP 382	461 (M) RTP 383
0 -0-CCH=CH- 590 (M) ATP 383	C=0 N-CH ₃ CH ₃ 1157(S) ATP 384	298(S) ATP 385	CH ₃ -C-CH ₃ CH ₃ 340(S) RTP 385
389 (H) HIT 303	1137137 117 304	230107 HII 303	C=0
CH-CI		-N-C-NH-	Ç-
828 (S) ATP 385	1033(S) ATP 385	1957(M) ATP 385	2050(S) ATP 385
-0	-¢-	-08 ₁₀ H ₁₀ C\$1 0- PARA	-CH ₂ -CH-CH ₂ -
24 (M) ATP 386	\$76(S) ATP 386	2014(M) ATP 386	66 (M) RTP 387
-ll-	с́=0 -сну_с —сну- сн ₂ ғ	<u></u>	-N-CH3
601 (M) RTP 387	788 (M) ATP 387	1030(S) ATP 387	1242(M) ATP 387

	сн ₃ -сн ₂ -ссн ₂ с=0	-CH=CH- TRANS TRANS 0=C C=0	CH=CH-TRANS
1629(M) ATP 388	148(M) ATP 389	689 (M) ATP 389	690(M) ATP 389
-¢сн ₂ сн ₂ -		-00404 ₂ - -0	-0-\$I
830 (M) ATP 389	851(S) ATP 389	973 (M) ATP 389	1152(M) ATP 389
-8-0-8-8-	0-0-	-HV	-CH ₂ -CH ₂
1261 (M) ATP 390	5(S) ATP 391	1061 (S) ATP 391	1913(M) ATP 391
CT-LV CT-LV		-CF	-2-
1914(S) ATP 391	319(S) ATP 392	711 (M) ATP 392	1064(S) ATP 392
0-		-CFCF_2-	-CF2-CF2-
1297 (M) ATP 392	1698(M) ATP 392	725 (M) ATP 393	997(M) ATP 393
0 -ссн=снс-	0 -0-C- TRANS	сн ₂ — сн-	-сн- сн ₂ вг
591 (N) ATP 394	1905(M) ATP 394	2180 (M) ATP 394	573(S) ATP 395

-0-P-0- -72	0 	CH ₂ -CH ₂ -CCH ₂ -	0 NH-C-
989 (M) ATP 395	990(S) ATP 395	1068(S) ATP 395	1593 (M) ATP 395
Ċ=0	CH ₂	-сн-	-C
1041(S) ATP 396	1290(M) ATP 396	2031 (S) ATP 396	93 (M) ATP 397
-×	CF2-CF2-	ርተ ²	L I I
1133(S) ATP 397	1063(M) ATP 398	71 (5) ATP 399	829(5) ATP 399
- с ғсн ₂ -сғ-	AH-	<u> </u> -c-	-00-
1124(H) ATP 399	1228(M) ATP 399	903(5) ATP 400	1071 (M) ATP 400
-cr ₂ -[cr ₂]_cr ₂ -	-HH-	-c	-oc
1421(M) ATP 400	1592(H) ATP 400	1904(M) ATP 400	87 (M) ATP 401
-C CF2 Cl	794 (M) ATP 401	1243(M) ATP 401	1292 (M) ATP 401
			

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	-HCH _Z CH _Z -	-cH2
2187(M) ATP 401	1254 (H) ATP 402	1255 (M) ATP 402
	-\$1CB ₁₀ H ₁₀ C\$1- PARA	-ÇF
1257 (M) ATP 402	. 2015(M) RTP 402	724 (M) ATP 403
-\$1св ₁₀ н ₁₀ с\$1- нетя	ÇF ₂	□ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □
1144(M) RTP 403	171 (M) ATP 404	185 (5) ATP 404
-0-51-0- 226 (M) ATP 404	C=0 CH- 232(S) ATP 404	CH ₂ CH—CH ₃ OH 1075(S) ATP 404
	C-NH-	-N+-C
1958 (M) RTP 404	1959 (M) ATP 404	104 (M) RTP 405
-0-6-		-CH
L17(M) ATP 405	124(M) ATP 405	995 (S) ATP 405
c=0 €1	5-	-
(038(S) ATP 405	1740(M) RTP 405	615(S) ATP 406

838 (5) RTP 406	1010(M) RTP 406	1260 (M) FTP 406
2003 (M) RTP 406	2197 (M) RTP 406	2203 (N) RTP 406
□ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □ □	CF2 CF2 CF2	CH ₃ -C-CH ₃ CH ₃ S09(S) RTP 407
1262 (S) ATP 407	1736 (M) ATP 407	1023(S) ATP 408
CI -00-0- 2005 (M) RTP 408	-CH _Z -CHCH _Z -OH OH 503(M) ATP 408	G54 (M) RTP 409
-141	₽	\$\langle \cdots
1238 (N) RTP 408	2010 (M) ATP 409	1775(M) ATP 410
205(M) RTP 411	207 (M) RTP 411	424 (H) ATP 412

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-SCCH ₂		CH2 CH2
556 (M) ATP 412	1602(M) ATP 412	679(S) ATP 413
782(S) RTP 414	CH ₃ CH ₂ CH ₂ S39(M) RTP 414	-0
N-N-NH-C-	₹3	
1239(M) RTP 414	367 (S) ATP 415	1039(S) ATP 415
-CH- CF ₂ CF ₂		-\$1\$1-
108(S) ATP 416	125(M) ATP 416	1151(M) ATP 416
-04 ₂ -0-	CH-CH-C	-CH ₂ -CHCH ₂ -
682(M) ATP 417	842 (M) ATP 417	856 (M)_ATP 417
	-CH2	CH2 1/2
959 (M) ATP 417	1218(M) ATP 417	1220(M) ATP 417
	s-	
1819(S) ATP 417	1844 (M) ATP 417	1024(S) ATP 418

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1530 (M) ATP 419	C=0 NH -C- 1 399(S) ATP 420	1603 (M) ATP 420
1697 (M) ATP 420	1777 (M) RTP 420	1855 (M) ATP 420
-0D1CH _Z	-CH2-CH-CH2-	-00-
708(M) ATP 421	-CH ₂ -N-CH ₂	1948 (M) RTP 421
684(S) ATP 422 C=0 1.056(S) ATP 423	1966 (M) ATP 422 C=0 NH CH ₃ 316 (S) ATP 424	2157 (M) RTP 422 -CH ₂ -CH-CH ₂ - F 1149 (M) RTP 424
		-o-l
438 (M) ATP 425	1824 (M) ATP 425	126 (M) ATP 426
L953 (M) ATP 426	394 (5) RTP 427	660 (K) RTP 427

C=0 F 187(S) ATP 428	CH ₂ CH ₂ CH ₂ CH ₂ L009(S) ATP 428	1040(S) ATP 428
1184(M) ATP 428	L185(H) ATP 428	1227(H) RTP 428
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1244 (M) ATP 428	1245(M) ATP 428	2200 (M) ATP 42B
274(S) ATP 429	1547(S) RTP 429	1809(M) ATP 430
-CH ₂ NCH ₂ C=0	634 (S) RTP 431	-SC-
1134 (M) ATP 431	2132(M) ATP 431	94 (M) ATP 432
101 (M) ATP 432	2169(H) ATP 432	95 (M) RTP 433

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\$ CH ₂ C N 745(S) ATP 433	2161 (M) ATP 433	CH2 CH2 CE N 743(S) ATP 435
1108 (M) RTP 435	663 (M) RTP 436	CHF CHF 820 (S) ATP 436
z m. – n. – n. – o. – o. – o. – o. – o. – o		
870(S) ATP 436	-CH ₂ -CHCH ₂	1817(S) RTP 436
2183(M) ATP 436	85 (H) ATP 437	1150(M) ATP 437
1110 (M) RTP 438	CH ₂ -CH ₂	0 0 1 1 -0
	-CH- CHCH ₃ CH ₃	-a12
955 (M) ATP 439	419(5) ATP 441	1642(M) ATP 441
- No No.		† <del> </del>
1695 (M) RTP 441	1918(M) ATP 441	355 (S) ATP 442

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	-h\( \)-NH-\( \)	<b>←</b>
1060(S) RTP 442	1937 (M) ATP 442	2044(H) RTP 442
481 (S) RTP 443	490 (M) RTP 443	2077 (M) RTP 443
The contraction of the contracti	012	
2154(M) RTP 443	2164 (M) ATP 443	243 (M) ATP 444
G-Z	-012 NH2	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
1846(M) RTP 444	1967(M)_ATP_444	1968 (M) RTP 444
	-01/2	CF ₂ -
1156(M) RTP 445	1639(M) ATP 445	1725(M) RTP 445
	-CH ₂ -CHCH ₂	, ch
130(H) ATP 446	172 (M) RTP 446	628 (S) ATP 446
	О В С С С	-ccH ₂ -c-
1543(S) ATP 446	2047(M)_RTP_446	174(M) RTP 447

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-CH ₂ -CHCH ₂ -	-ç	-0-CH- -0-CH ₃
756 (M) ATP 447	970 (M) ATP 447	2115(H) ATP 447
CH-CH ₃ 2116(S) RTP 447	-ţ	1985 (M) RTP 448
	-NH-CH ₃	
2188(M) ATP 448	563 (H) RTP 449	1120(M) ATP 449
1121 (N) 878 448	N N N N N N N N N N N N N N N N N N N	-ss 642 (M) ATP 451
L121(M) ATP 449	1857 (M) ATP 450	642 (F) HIF 451
-0 CH ₃ CH ₃	-0-2	
678(M) ATP 451	242 (M) ATP 452	1205 (M) ATP 452
CH ₂		-c
1208 (M) ATP 452	1929 (M) ATP 452	1930 (M) ATP 452
-0		<b>←</b>
840 (M) RTP 453	L535(M) ATP 453	1730 (M) ATP 453

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	0-CH ₂
2149(H) RTP 453	349(S) RTP 454
-NHNH-	
1161 (H) ATP 454	2205 (H) RTP 454
CH ₃ CH ₂ CH ₃ CH ₃ 2206 (N) RTP 454	CH ₂ CF ₂ CH ₂ CH ₂ CH ₂ CHF ₂
111 101	THE TOO
-0	-NHCH ₂ CF ₂ -
1645 (M) ATP 455	197(M) RTP 456
	-\$1\$1-
1849(N) ATP 456	965 (M) ATP 457
NH-	
1573(M) ATP 457	1871 (N) ATP 457
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1872 (N) ATP 457	2174 (M) RTP 457
;=0 CH2 -;—	сн ₂ -сн ₂ - с≕о
616(S)_RTP_458	807 (H) ATP 458

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-ch2-chch2-	-0	
860 (H) RTP 458	991 (M) ATP 458	1119 (M) RTP 458
-NH-CT-	5-	CH3
1190(N) ATP 458	1811(N) ATP 458	1919(M) ATP 458
The CHY		
1998(N) ATP 458	2182(N) ATP 458	623 (S) ATP 459
2190(M) ATP 459	667 (N) RTP 460	1634 (M) ATP 460
-N- C=0 \f2 1141(S) ATP 462	-CH ₂ -N-CH ₂ - 0 0 1600 (M) ATP 462	NH-C-
1677 (M) ATP 462	-CH ₂ -CH ₂ -CH ₂ -CH ₂ -1992 (M) ATP 462	2123 (M) ATP 462
	NH-c-	
2137 (M) RTP 462	1921 (M) ATP 463	1001(S) RTP 464
	-cf ₂ cfcf ₂ - cf ₃	-o\$-
2086 (N) ATP 464	792 (H) ATP 465	1107 (M) RTP 465

		,
-0-CH ₃		
1154 (H) ATP 465	1988(M) ATP 465	2199(M) ATP 465
CH ₂ 420 (S) RTP 466	CH- CH ₂ 631 (S) ATP 466	CH ₂ CH ₂ 664 (S) RTP 466
420137 HII 400	031(37 H11 488	004137 RT 488
	CH3-C-CH3	
665 (H) RTP 466	696 (5) ATP 466	2084 (M) RTP 466
-NHNHC-	-CH _Z -CFCH _Z - C=0	CF ₂ -
1229 (N) ATP 467	817 (M) ATP 468	1851 (M) RTP 468
CH3 CH3		○
657 (N) ATP 469	2085(N) ATP 469	1116(M) ATP 470
1117 (N) RTP 470	-CH ₂ -CH ₂ -	2087 (M) ATP 471
11111111 HIL 7/0	2501 (III 710	20071117 1711 771
	-0-\N=N-	
2198(M) RTP 471	1109(M) RTP 472	1250(M) ATP 472
-N-1	CF2 CF5	-C
1985 (M) ATP 472	1012(S) ATP 474	1072(M) ATP 474

		
	-NH-NH-NH-	- C
1114(M) RTP 475	1693 (M) ATP 475	1945(M) ATP 475
1946(M) ATP 475	2018(M) ATP 475	2019(M) ATP 475
-o-Ē-Ç	-N-0-0F2-	TRANS
733(H) ATP 476	2024 (M) ATP 476	1259 (M) ATP 477
-0	JERUM OTR 477	
1268 (H) ATP 477	1694 (M) RTP 477	2196 (M) ATP 477
-CH ₂ -SI-CH ₂ -		-00-
607(H) ATP 478	1098(M) ATP 478	1099 (M) ATP 478
N-CH ₃	HH-C-	-CH2 OH2 CH2
1692(S) ATP 479	1187 (M) ATP 480	1915(M) ATP 481

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CH3		-GF- C==0 0
2128(H) ATP 481	2191 (M) ATP 481	193 (S) ATP 482
-0	-¢- CH2	-N-CH2-N-
430(N) ATP 482	1068(S) ATP 482	1994 (M) ATP 482
		-N
2131 (M) ATP 482	844(S) RTP 483	1137(S) ATP 483
		CH2
2194 (M) ATP 483	1986 (M) ATP 484	681 (S) ATP 485
	010	9 - \$сн₂- ç
1502 (M) ATP 487	1504 (M) ATP 487	2046 (M) ATP 487
	-NHCH2-	0 CH ₂ CH ₂
1230 (M) ATP 488	1231 (M) ATP 488	1912(M) ATP 489

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396 (S) ATP 490	1249(M) RTP 490
	-0-CH ₃
1282 (H) RTP 490	2117(M) ATP 490
410(S) RTP 491	-C
- CH ₂ - CH ₂ - Cl	
330 (M) RTP 492	668 (M) ATP 492
953 (M) ATP 492	-NH-C
2173(H) RTP 492	1272(M) RTP 493
	NO _Z
1949(M) ATP 493	1025(S) ATP 491
1200(H) RTP 494	1202(M) ATP 494

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ĊH ₂		
1174(S) ATP 495	1859(M) ATP 495	2078 (M) ATP 495
S-	-NH-C-	S -NHNH
1196(M) ATP 496	1950(M) ATP 496	2048(N) ATP 496
-N-NH-E-		
2052(M) ATP 496	2152(M) ATP 496	1542(S) RTP 497
	-N-CH ₂ -	CH ₃ -CB ₁₀ H ₁₀ CSIO- METR CH ₂
1580(M) ATP 497	1987(M) ATP 497	969 (M) ATP 499
	N NH-	
1947(M) ATP 499	1804(M) ATP 500	1558(S) ATP 501

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1933(M) ATP 501	2148(H) ATP 501
- E	
1226 (H) RTP 502	1867(H) RTP 502
Ċ≔0 N~-CH ₂ - CH ₂	-0-0-
400 (S) ATP 503	1094(M) ATP 503
F	-NBH
1153(M) RTP 503	1236(H) ATP 503
C Care	
1295 (M) ATP 503	1623(M) ATP 504
	- CH ₃
1274(H) RTP 505	1721 (M) ATP 505
C=0 NH CH ₂ 393 (S) ATP 506	910(S) ATP 506
	-n-NHc-
1251(M) ATP 506	1939(M) ATP 506

TK BBU4

		,
2185(M) ATP 506	1648(M) ATP 508	1671 (S) ATP 508
1 CH2 CH2	-0	
748(S) RTP 509	1118(M) ATP 510	1283(M) ATP 510
	-0-0-0-0	-0+ -0- -0-
1813(N) ATP 510	666 (M) ATP 511	1172(S) ATP 511
1690(M) ATP 511	95 (M) ATP 512	C=0 NO ₂ 1027(S) ATP 512
	-N_N-C-CH ₂ -	-\$
2008(N) ATP 512	437(M) ATP 513	641 (M) ATP 513
TRANS CH ₃		CI
1258 (M) ATP 513	1553(S) ATP 513	1057(S) ATP 514

2186 (M) ATP 514	296(5) ATP 516
-ç	-NH-N N-C-
1096(M) ATP 516	1936(M) ATP 516
97 (M) ATP 517	1617(M) ATP 517
-0	CH3 CH3
1999(M) ATP 517	2089(M) ATP 517
N-CH ₂ -CH ₂ -	1727 (M) ATP 518
1860(M) ATP 518	-CF ₂ -CF-CF ₂ - F 195(M) ATP 519
	-NH-CH3
1973(M) ATP 520	2133(M) ATP L20
	-1-2
1281 (M) ATP 523	1927(M) ATP 524

		
-1	O Eliz	NH-C-
1928(H) ATP 524	206(S) ATP 525 '	1082 (H) ATP 526
1505(M) ATP 528	1506(M) ATP 526	1831 (S) ATP 526
1608(N) ATP 527	1977(H) ATP 527	2202 (M) ATP 528
		-NH—с—сн ₂ -
1566(M) ATP 529	1279(M) ATP 530	15 (M) ATP 531
00!		о -ёNHСН ₂ -
799 (M) ATP 531	1863(N) ATP 531	11(M) ATP 533
		-C- -C- -C-
1139(5) ATP 533	1978 (M) ATP 533	189(S) ATP 534

986 (S) ATP 535	1115(M) ATP 535
CH—CH ₃ CH ₃ CH ₃ 671 (S) ATP 536	2148 (H) ATP 538
2207 (M) ATP 536	2187(M) ATP 537
1940 (H1 RTP S38	2049 (H) RTP 538
1975 (M) ATP 540	1285(M) RTP 541
1288 (M) RTP S41	1981 (H) RTP 541
2130(M) ATP 541	1644 (M) ATP 544
CH-CH-CH2	
843 (M) RTP 547	1225(M) ATP 548

1681 (M) ATP 548	1683(S) ATP 548
2143(M) ATP 548	1267 (M) RTP 549
1650 (M) ATP 549	2175(M) ATP 549
2176(M) ATP 549	2178 (M) ATP 549
	- <u>F</u>
2192(M) ATP 550	1175(S) ATP 551
-181-	
1678 (M) ATP 551	2166 (M) ATP 551

		,
2021 (M) ATP 552	9 -5NHCH ₂ - 0 2022 (M) ATP 552	175 (S) ATP 554
		CF2-
1980(M) RTP 554	1753 (M) ATP 555	2041 (M) ATP 555
		-NHNNH-
1101(M) ATP 556	2063(H) ATP 556	1938 (M) ATP 557
	-101-1-101-	
1628 (M) ATP 558	1234(M) ATP 559	1845 (M) ATP 559
	NH-	2000 (N) 550 550
1670(M) ATP 560	1801 (M) ATP 560	2098(M) ATP 560
		\leftarrow
2208 (M) ATP 560	2209(M) ATP 560	2043(M) ATP 561
\$\frac{1}{4}		
1733(M) RTP 562	6(S) ATP 563	1523 (M) ATP 563

O C C C NO2		
1906 (M) ATP 563	730(H) ATP 565	1540(M) ATP 565
	-c-N-c-	CH ₂
1544(S) ATP 565	1916 (M) RTP 565	1293 (M) ATP 566
-I CH ₂		-\$1
1979 (M) ATP 566	408(S) ATP 567	1717(M) ATP 569
-CH2-CH-CH2-		
904(M) ATP 571	1171(S) ATP 571	1703(M) ATP 571
		F=0
1633 (M) ATP 575	1581 (M) ATP 576	1582(S) ATP 576
1679 (M) ATP 577	2126(M) ATP 578	781 (S) ATP 579

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1270 (M) ATP 579	1277 (M) ATP 579
1920(S), DTP 570	
1829(S) ATP 579	2171 (M) RTP 579
2172(M) ATP 579	721 (M) ATP 580
CH ₃	
722(M) ATP 580	1103(M) ATP 580
1122 (M) ATP 580	2073 (M) ATP 580
737(M) ATP 581	1201 (M) ATP 583

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	- C
1858(N) ATP 584	1591 (M) ATP 586
1086 (M) ATP 589	CH ₂ 698 (S) ATP 590
CIF ₂	
2040 (M) ATP 590	2150(M) ATP 591
-NH-NN-NN-NN-NN-NN-NN-NN-NN-NN-NN-NN-NN-	-E-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-
1803 (N) ATP 595	1578 (M) ATP 596
1513(M) ATP 597	1559(S) ATP 597
	-CC
1878 (M) ATP 597	109(H) ATP 589

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<b>←</b>	-l	<b>₹</b>
100 (M) ATP 600	142 (N) ATP 600	1093(N) ATP 600
		CH ₃
1700(H) ATP 600	1701(M) ATP 600	2193(N) ATP 600
1194(M) ATP 602	1621(M) RTP 602	1508(M) ATP 605
	N-CH ₂	
2127(M) ATP 805	1663(S) ATP 606	2111(N) ATP 606
2210 (N) ATP 606	2211 (M) ATP 606	1594 (M) ATP 607

	T
NH CHCH ₃ CH ₂ 395(S) ATP 608	1276 (M) ATP 608
1760(M) ATP 608	2061 (M) ATP 609
1630(M) ATP 613	1181(M) ATP 614
1536(S) ATP 616	2067 (M) ATP 616
	_
2068(M) ATP 616	1583(M) ATP 617
2163(M) ATP 617	1269 (M) ATP 620
L613(M) ATP 621	1597(M) RTP 624
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1827(S) ATP 627	1085 (M) ATP 628
CF ₂ -CF ₂ -	1825(S) ATP 631
-CH ₂ -N-CH ₂ -	-CH- C=0
2080 (M) ATP 635	2081 (M) ATP 637
1691 (M) ATP 642	2062 (M) RTP 645
O CH2 C-	-\-\-\-\-\-\-\-\-\-\-\-\-\-\-\-\-\-\-\
1874(M) ATP 647	2075(M) ATP 649
980(S) ATP 651	1780(M) ATP 659

2165 (M) ATP 659	1879(M) ATP 663
1604 (M) ATP 664	1084 (M) ATP 665
-NI	
1561 (M) ATP 565	1287(M) ATP 666
1549(S) ATP 668	1271 (M) ATP 669
1989 (M) ATP 673	1990 (M) ATP 673
N N N	1880(H) HIF 0/3
1551 (S) ATP 675	1612(M) ATP 676
	~ N—cH₂
1982 (M) ATP 678	1983(M) ATP 678
	- <del></del>

1984 (M) RTP 678  1726 (M) RTP 684  1873 (M) RTP 684  1626 (M) RTP 685  1016 (M) RTP 690  1503 (M) RTP 690  -CH2_CH-CH2_	
1873 (M) RTP 684  1626 (M) RTP 685  -NH-C-  1016 (M) RTP 690  1503 (M) RTP 690  -CH ₂ -CH-CH ₂ -	_
1873(M) RTP 584  1626(M) RTP 585  -NH-C	
1016(M) ATP 690  1503(M) ATP 690  -CH ₂ -CH-CH ₂	
-CH _E -OH-CH _E	
2060 (M) ATP 693 373 (M) ATP 695	
2000 117 111 000	
1275 (M) ATP 695	
1273(M) RTP 705 2074(M) RTP 713	
1800 (M) RTP 714 (527 (M) RTP 717	

1180 (M) ATP 719	1278(M) ATP 720
1203(M) ATP 724	2079(M) ATP 724
1235(M) ATP 725	1766 (M) ATP 727
2017 (M) ATP 730	1669 (M) ATP 736
-0-1264 (M) ATP 739	1280 (M) ATP 739

1702 (M) ATP 740	2168 (M) ATP 740
-c	N-CH _Z -CH _Z
1708(M) ATP 741	2066 (M) ATP 755
738 (M) ATP 758	1673 (M) ATP 781
1772(M) ATP 783	2093(M) ATP 787

\$ CH2	N NH-CH ₂
2144(M) ATP 787	1660(M) ATP 806
1500(M) ATP 823	2065(M) ATP 825
1565(M) ATP 837	1298(M) ATP 861
CH2	CH ₂
1761 (M) ATP 865	1783(S) ATP 891
СН2—СН2	OT TO-01-2
1197(M) ATP 1043	2139(M) ATP 1043

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1215 ATP 350

1218 ATP 417

2143 ATP 548

1226 ATP 502

GROUPS IN NUMERICAL ORDER OF ATP WITHIN HIERARCHICAL ORDER OF MAIN SINGLE-GROUP

1180 ATP 719	-CF ₂ -CF ₂ -
1185 ATP 428	-NH
2080 ATP 693	2139 ATP 1043
1103 ATP 580	1201 ATP 583
CH2	-cH2-1 CH2

1211 ATP 360

1205 ATP 452

2144 ATP 787

1238 ATP 409

1263 ATP 344	1260 ATP 406
-0	
1264 ATP 739	1271 ATP 669
1280 ATP 739	1278 ATP 720
1287 ATP 666	1502 ATP 487

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	-CH ₂ -N-CH ₂ -
1505 ATP 526	1299 ATP 633
1500 ATP 823	2148 ATP 501
1580 ATP 497	1586 ATP 529
2166 ATP 551	1540 ATP 565
$\stackrel{\sim}{\sim}$	~
2150 ATP 591	1578 ATP 596
2067 ATP 616	1583 ATP 617
	-NH-NH-
2065 ATP 825	1592 ATF 400
1591 ATP 586	1594 ATP 607

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2061 ATP 609	1597 ATP 624
CH ₂	CH ₃ CH ₂
1290 ATP 396	1293 ATP 566
1604 ATP 664	1621 ATP 602
1004 HIF 004	1021 HIF OUZ
1613 ATP 621	1612 ATP 676
1634 ATP 460	1628 ATP 558
	-CH ₂ -N-CH ₂ -
1602 ATP 412	1600 ATP 462

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-012	-CH2	-0
1642 RTP 441	1639 RTP 445	1645 ATP 455
1648 ATP 508	1650 ATP 549	2208 RTF 560
The contract of the contract o		
2210 RTP 606	2165 ATP 659	2158 RTP 740
		CH ₂
2175 ATP 549	2209 ATP 560	2073 ATP 580
2211 ATP 806	1766 ATP 727	1772 ATP 783
Cast fill GVG	TIME CITE 121	ATTE 1111 199
	CF ₂	
1736 RTP 407	1725 ATP 445	1730 ATP 453

2123 ATP 462	1691 ATP 548	1753 ATP 555
1733 ATP 562	-51 - 0 1717 ATP 569	1086 ATP 589
2040 ATP 590	1084 ATF 665	1708 ATP 741
CH3		CF ₂
722 ATP 580	737 ATP 581	1846 RTP 444
1851 ATP 468	2128 ATP 481	1860 ATP 518
1863 ATP 531	2167 ATP 537	2126 ATP 578
2172 ATP 579	2127 ATP 605	2079 ATP 724
2171 ATP 579	1867 ATP 502	2130 ATP 541

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000	-0F ₂ -0F ₂	-CF ₂ -CF ₂ -	-0-N-O-
1871 ATP 457	594 RTP 277	595 ATP 305	1812 ATP 371
-0F	-ÇF	-ÇF	
528 ATP 372	711 ATP 392	725 ATP 393	724 RTP 403
NI			NH2
1683 ATP 475	1859 ATP 495	1845 ATP 559	1803 ATP 585
	- No. 10 - N	-Net-Net-2	-NOTNOTNOT
1700 ATP 600	1661 ATP 665	1800 ATP 714	1695 ATP 441
	CH2 CH2	-012-012-012	-CH ₂ -D-CH ₂
1857 RTP 450	1913 ATP 391	1915 ATP 481	1873 ATP 684
-0	Nac Can	CH3 CH3 CH3	TRANS CH3
1094 ATP 503	1251 ATP 506	1956 ATP 356	1258 ATP 513

CH ₃ 0	CH ₃	0 L ₃
-NH-N N-C-	-NH-N N-NH-	
CH ₃	CH ₃	CH ₃
1936 ATP 516	1938 ATP 557	1916 ATP 565
-cH ₂ -N-CH ₂ -		-NHNNH
1942 ATP 300	438 RTP 425	1953 RTP 426
₩ C-E-	-0-F	-s-NH-
1250 RTP 472	144 RTP 325	1962 ATP 69
-1		
1958 RTP 404	2200 ATP 428	2174 RTP 457
		-CH _Z -N -CH _Z
2199 RTP 465	2146 ATP 536	1966 RTP 422
-012-N-C-	-C	-C
1255 ATP 402	1928 ATP 524	1930 ATP 452
1970 ATP 169	-CH ₂ -CH ₂ -CH ₂	1122 ATP 580
1973 ATP 520	1977 ATP 527	1978 ATP 533

	-c- <del>y=\-</del> c-
- N - N	N N
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1976 ATP 540	1919 ATP 458
-c	-cH ₂ -N-CH ₂ -
СH3	Ö NH
1926 ATP 298	1991 ATP 301
	NH CH2
1986 ATP 484	1989 ATP 673
1980 ATP 554	1983 ATP 678
1300 HT 334	1303 Hil 010
-0 C C C C C C C C C C C C C C C C C C C	
2008 ATP 512	1999 ATP 517
-cH ₂ -CH ₂ -	0-\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
1992 ATP 462	1781 ATP 865
2017 ATP 730	1879 ATP 663
-0-0-0-	
1948 ATP 421	730 RTP 565

-cH ₂ CH ₂ -CH ₃	-CH ₂ -CH ₂ -	-\$1—СВ ₁₀ Н ₁₀ С —\$1- МЕТЯ
658 ATP 275	655 ATP 337	1144 RTP 403
-\$1CB ₁₀ H ₁₀ C\$1- PARA	-\$ıCB ₅ H ₅ C\$ı-	-\$ı-0-\$ı-
2015 ATP 402	675 ATP 355	874 ATP -52
-c-o- <del>-</del> b+-	П -Росн ₂ -	-сн ₂ -осн ₂ -
1000 ATP 58	975 ATP 132	99 ATP 174
—N—0—cF _Z -	-çғocғ ₂ -	о -сосн ₂ -
962 ATP 177	433 ATP 177	103 ATP 193
	- <del>сн-о-сн₂-</del>	-cr ₂ ocr ₂ -
454 ATP 239	707 ATP 244	452 RTP 246
-CF ₂ 0CH ₂ -	-c-a-c-	-CH _Z -
159 ATP 248	90 ATP 254	1400_ATP_258
-CH ₂	-сносн-	F N 0-CH ₂
1301 ATP 267	930 ATP 309	816 ATP 325
F 0-CH ₂		
141 ATP 325	2016 RTP 343	2011 ATP 346
0-6-	-ç॑осн ₂ -	
1008 RTP 346	877 ATP 352	1738 ATP 355

801 ATP 357  541 ATP 373  1261 ATP 390  F O CH _Z 2203 ATP 406  2003 ATP 406  2003 ATP 406  2005 ATP 417  1855 ATP 420  1245 ATP 428  2044 ATP 442  1156 ATP 445  2188 ATP 448  2182 ATP 458  2190 ATP 459  2019 ATP 475  2024 ATP 476  2191 ATP 481  2195 ATP 506  1813 ATP 510  97 ATP 517			
2203 ATP 406  2003 ATP 406  2003 ATP 406  2015 ATP 411	0-0-	0-CH ₂	-8-0-8-8-
2203 ATP 406  2003 ATP 406  2003 ATP 406  2005 ATP 411	801 ATP 357	541 ATP 373	1261 ATP 390
CH ₂ -0-C-  682 ATP 417  1855 ATP 420  1245 ATP 428  2044 ATP 442  1156 ATP 445  2188 ATP 448  2205 ATP 454  2182 ATP 458  2190 ATP 459  2019 ATP 475  2024 ATP 476  1098 ATP 478  2191 ATP 481  1347 ATP 499			F -0-CH ₂ -
682 ATP 417  1855 ATP 420  1245 ATP 428  2044 ATP 442  1156 ATP 445  2188 ATP 448  2182 ATP 458  2190 ATP 459  2019 ATP 475  2024 ATP 476  2191 ATP 481  2191 ATP 489  2191 ATP 489	2203 ATP 406	2003 ATP 406	205 RTP 411
2044 ATP 442  1156 ATP 445  2188 ATP 448  2205 ATP 454  2182 ATP 458  2190 ATP 459  2019 ATP 475  2024 ATP 476  2191 ATP 481  21947 ATP 499	-CH ₂ -0		
2044 RTP 442  1156 RTP 445  2188 RTP 448  1995 RTP 448  2205 RTP 454  2182 RTP 458  1995 RTP 459  2019 RTP 475  2024 RTP 476  1996 RTP 478  2191 RTP 481  1947 RTP 499	682 ATP 417	1855 ATP 420	1245 ATP 428
1995 RTP 448  2205 RTP 454  2182 RTP 458  0 -5-0-0 0 2190 RTP 459  2019 RTP 475  2024 RTP 476  1098 RTP 478  2191 RTP 481  1947 RTP 499	~~~~~		
1995 RTP 448  2205 RTP 454  2182 RTP 458  0 -5-0-0 0 2190 RTP 459  2019 RTP 475  2024 RTP 476  1098 RTP 478  2191 RTP 481  1947 RTP 499	2044 ATP 442	1156 RTP 445	2188 RTP 448
2190 ATP 459  2019 ATP 475  2024 ATP 476  2024 ATP 476  1098 ATP 478  2191 ATP 481  1947 ATP 499			
2190 ATP 459  2019 ATP 475  2024 ATP 476  1098 ATP 478  2191 ATP 481  1947 ATP 499	1995 ATP 448	2205 ATP 454	2182 ATP 458
1098 ATP 478  2191 ATP 481  1947 ATP 499		-5=-0 -5=-0	0 -N-0-CF ₂ -
1098 ATP 478  2191 ATP 481  1947 ATP 499  0 -0-c- 1098 ATP 478  1947 ATP 499	2190 ATP 459	2019 ATP 475	2024 ATP 476
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	1098 ATP 478	2191 ATP 481	1947 ATP 499
2185 ATP 506 1813 ATP 510 97 ATP 517	* ~ ~ *		
	2185 ATP 506	1813 ATP 510	97 ATP 517

2202 ATP 528	1265 ATP 541
1267 ATP 549	2043 ATP 561
0 0	
	-o-c-
1270 ATP 579	109 ATP 599
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1093 ATP 600	100 ATP 600
1269 ATP 620	1726 ATP 684
1764 ATP 280	2183 ATP 436
-ch ₂ -sch ₂ -	
2047 RTP 446	667 ATP 460

2018 ATP 475	2186 ATP 514
2049 ATP 538	2176 ATP 549
COOL OTE STO	
2021 ATP 552	1878 ATP 597
	-çнsсн ₂ -
1108 ATP 435	546 ATP 115
-CF ₂ SCF ₂ -	-s—s—сн ₂ -
643 ATP 131	538 ATP 165
-CH2-S-CH2	578 ATP 214
S N	-ss
2201 ATP 237	545 ATP 246
0 == -сs _с н-	о -с-sсн ₂ -
1909 ATP 320	424 RTP 412

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-\$-cH ₂ -	-SS-	-N=	C: -N=
101 RTP 432	541 ATP 513	162 ATP -72	441 ATP 160
-N=N=N=	NH -N=	Br -N= -N= - 	NH -N=
637 ATP 205	796 ATP 209	824 ATP 259	822 ATP 352
N- -N	-N==PF2N==PF2N==PF2-		-0NCF ₂ - CF ₂
644 ATP 378	770 ATP 169	1110 ATF 438	981 ATP 237
-0-NCF ₂ - CF ₃	-C	-cNcH2- CH2	-c
33 ATP 284	706 ATP 301	699 ATP 311	1240 ATP 347
-\$1\$1- -\$1-	N-CH ₃	-CH ₂ NCH ₂ - C=0	M N N N
610 ATP 350	1242 RTP 387	1134 ATP 431	1856 ATP 584
-CH ₂ -NHCH ₂ -	NH -C-	NH-C-	-\$1-NH-\$1-
519 ATP 0	561 ATP 52	1963 ATP 69	602 ATP 321
N_N-NH-C-	NH- E-	5-NH-C-	-N-NH-
1955 ATP 357	1593 ATP 395	1239 ATP 414	1937 ATP 442
NH-C	NH-C-	-NHNHC-	N NH
1676 RTP 462 '	1921 ATP 463	1229 RTP 467	1694 ATP 477

		,
NH-C-	-NH-C-	-N-NH-C-
1187 ATP 480	1230 ATP 488	2052 ATP 496
NH-C-	F NH-C-	-ймнЁ-
1950 ATP 496	1153 ATP 503	1939 ATP 506
N NH NH	NH-C-	0 -С—NH—СН ₂ -
1690 ATP 511	1082 ATP 526	11 ATP 533
-9NHCH ₂ -	NH-C-	
2022 ATP 552	1235 ATP 725	1669 ATP 736
NH-CH ₂	-a- a-	
1660 ATP 806	968 ATP 271	994 ATP 374
-0-F-0- CF2	-0	-0-1-0-
989 ATP 395	992 ATP 431	991 ATP 458
СН _З NH\$1NH СН _З	СН _З -СН _Z -\$1—СН _Z - СН _З	CH ₃ -0-5:CH ₂ - CH ₃
508 ATP 151	588 ATP 157	297 ATP 181
CH3 -0-\$1-0- CH3	CH3 -CB5H5C-51-0- CH3	CH3 -0-\$1-CH2- CH2
223 ATP 209	676 ATP 226	467 ATP 231

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CH3	-CH ₂ -\$1CH ₂	-CH ₂ -51-CH ₂ -
608 ATP 240	759_ATP 249	603 ATP 252
CH3 -0-\$1-0-	-0-51-CH3	-0-\$1 CH ₃
266 ATP 259	710 ATP 265	25 ATP 271
-0-51 F	CH3 -0-\$1-0- -CH2	СН ₃ -СВ ₅ Н ₅ С\$;о- ГН ₂
460 RTP 273	263 ATP 319	888 ATP 325
CH ₃ -CB ₁₀ H ₁₀ C - SI - O- META CH ₃	CH ₂ -0-51-0- CH ₂ 521 ATP 333	1723 ATP 341
1143 HT 327	321 HT 333	1723 H11 341
CH3 -0-\$1-0-	CH3 -C8 ₁₀ H ₁₀ C - \$1 - C8 ₁₀ H ₁₀ C - METR CH3 METR	CH3 -0-5; -0-
462 ATP 353	2013 ATP 367	734 ATP 374
CH3 -C8 ₁₀ H ₁₀ C —\$1 —0- PARA CH ₃		
2014 ATP 386	1152 ATP 389	226 ATP 404

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-0	CH- -0-CH ₃	-¢
207 RTP 411	2115 ATP 447	970 ATP 447
-0	-ç	-Ę
2117 ATP 490	1096 ATP 516	490 RTP 443
-l	-NH-	CH ₃
125 RTP 416	574 RTP 207	2179 ATP 350
-NH-CH ₃		-00-
563 ATP 449	483 RTP 293	905 ATP 345
	- G-F2	-00-
CH ₃ 1017 ATP 348	1010 ATP 406	1154 ATP 465
-CCC		-0-0-
1072 ATP 474	2196 ATP 477	1099 ATP 478
-CC	-66-	
1906 ATP 563	1581 ATP 576	124 ATP 405
-aa		-NH-CH3
2005 ATP 408	955 ATP 439	2133 ATP 520

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1946 ATP 475	1256 ATP 541	1780 ATP 659
N-N		-9
1969 ATP 168	1765 ATP 280	1763 ATP 280
	-042 042	-\$1CF ₂ -
1770 ATP 307	44 ATP 308	127 ATP 333
-0-CF ₂ -		-CF ₂ -CF ₂ -
800 RTP 342	2113 ATP 346	157 ATP 377
-0-0-		-C
1071 ATP 400	2187 ATP 401	794 ATP 401
	-\$1\$1-	
2197 ATP 406	1151 ATP 416	2169 RTP 432
	-0	
2161 ATP 433	95 ATP 433	243 RTP 444

1121 ATP 449 2149 ATP 453
2137 RTP 462 2086 RTP 464
2084 ATP 486 1272 ATP 493
1727 RTP 518 2078 RTP 531
2207 ATP 536 2178 ATP 549
2041 ATP 555 1234 ATP 559
2080 ATP 635 1691 ATP 642

1503 ATP 690	2066 ATP 755
-00-0- 673 ATP 162	2058 ATP 175
-0S 1112 ATP 218	-0-NH- 1237 ATP 229
-0-CH ₂ -	2184 ATP 237
-0	1774 RTP 291
-0—Сн- 115 ATP 291	1531 ATP 297
-\$1CF ₂ -	2158 ATP 315
-0-C- 92 ATP 326	1790 ATP 329
CH ₂	
1866 ATP 330	1611 ATP 336

		
-CH ₂	0-	-NH
539 ATP 350	1620 ATP 352	1761 ATP 3S6
\$1-	GI NH-	-o
1724 ATP 363	1762 ATP 376	24 ATP 386
		0-
1629 ATP 388	1297 ATP 392	1698 ATP 392
-c-<	NH-	-h-
93 ATP 397	1292 ATP 401	1243 RTP 401
0 N-C-5- 1740 RTP 405	2010 ATP 409	1775 ATP 410
-0-	\$\frac{1}{2} \rightarrow 5-	0-
1113 ATP 414	1844 ATP 417	959 ATP 417
1530 ATP 419	1603 ATP 420	1777 RTP 420
N-CH ₂		
1697 RTP 420	2157 RTP 422	1824 ATP 425
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660 ATP 427	2160 ATP 430	1809 ATP 430

-s	1102 RTP 436	2077 ATP 443
	-s	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
1120 ATP 449	642 ATP 451	1535_ATP_453
-a	NH-NH-	0-
840 ATP 453	1573 ATP 457	1872 ATP 457
	5-	CH ₂
965 ATP 457	1811 ATP 458	1998 ATP 458
-0S		
1107 ATP 465	665 ATP 466	2085 ATP 469
1117 ATP 470	2198 ATP 471	2067, ATP 471
-N	-0	2131 ATP 4882
	-c	
1282 ATP 490	996 ATP 491	2173 ATP 492
-0-		5-
668 RTP 492	1202 ATP 494	1196 ATP 496
-NH CH2	NH-	N-042
1987 ATP 497	1804 ATP 500	1295 ATP 503

-NH	
1236 ATP 503	1623 ATP 504
1274 ATP 505	1283 ATP 510
12/4 HIF 505	1283 HIF SIV
1118 ATP 510	-0
	555 mi 511
1617 ATP 517	1281 ATP 523
1608 ATP 527	1278 ATP 530
Q Q	
1981 ATP 541	1644 ATP 544
-0	2192 ATP 550
-NH-	
1678 ATP 551	2098 ATP 560
AGEO OVER 550	
1670 ATP 560	1523 ATP 563
-N	
1979 ATP 566	1703 ATP 571

1633 RTP 575	1679 ATP 577
1277 ATP 579	721 ATP 580
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-CC	1194 ATP 602
1508 ATP 605	1276 ATP 608
1780 ATP 808	1830 ATP 613
1181 ATP 514	2068 ATP 616
2081 ATP 637	2062 RTP 645
1990 ATP 673	1984 ATP 678
1626 ATP 585	1507 ATP 695

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1527 ATP 717	1203 ATP 724	1501 ATP 753
NH O-		CH ₃ CH ₂
738 ATP 758	1565 ATP 837	2206 ATP 454
CH ₃	C C C C C C C C C C C C C C C C C C C	-¢
953 ATP 492	663 ATP 436	952 ATP 448
	-ss-	-сн-
130 ATP 446	579 ATP 214	1116 ATP 470
TRANS	-CH ₂	-ĒĒ
1904 ATP 400	1233 ATP 324	601 ATP 387
СН ₂ -СН ₂ -	-NH	-CH=CH
1206 ATP 452	1231 ATP 488	1162 ATP 305
-CH=CH	-CH=CH- TRANS TRANS 0=C C=0	-CH=CH
1168 ATP 353	689 ATP 389	1164 ATP 256
-cH=CH- Q	-cH=CH- CH=CH-	-042-0=04-042 CIS
1166 ATP 271	1167 ATP 362	304 RTP 203

-042-C=04-042- C13	CH ₃ -CH ₂ -C=CH-CH ₂ - TRANS	CI    -CH ₂ -C=CH-CH ₂ - TRANS	- <del>012-</del> CH=CHCH2- CIS
304 ATP 203	307 RTP 268	139 ATP 303	120 ATP 266
-сн— <del>сн—сн_</del> сн—сн ₂ -	CH=CH-CTS	-CH2-CH=CHCH2- TRANS	CH=CH-CH-TRANS
377 ATP 288	1163 ATP 305	121 ATP 277	690 ATP 389
	CH=CH-Ch	-ссн=-снс-	-ŅCCH2-
1165 ATP 99	1169 ATP 353	591 ATP 394	704 ATP 169
-acNH-	-00	-o-c-cਮਣ ਹੈ	-\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
445 ATP 202	177 ATP 218	178 ATP 232	3 ATP 238
-0CCF ₂ -		-N-C	-scp+-
596 ATP 257	1920 RTP 265	1925 ATP 298	1911 ATP 320
-N-C-O-	-00-	-NHCNH-	
1004 ATP 329	110 ATP 347	1954 ATP 357	1710 ATP 360
-N-C-CH ₂	-a-c	-0Ca=a-	
1917 ATP 366	599 ATP 368	590 ATP 383	1957 ATP 385
-0-C-TRANS		-o-c-	
1905 ATP 394	1228 ATP 399	87 ATP_401	1257 ATP 402
C-N+	-0-6	-NH-C-	-s-с-сн ₂ -
1959 ATP 404	117 ATP 405	104 ATP 405	556 ATP 412
-0-C	-0-	- N-	-occ-
126 RTP 426	1244 RTP 428	1227 RTP 428	544 ATP 439

	CC	0-6-0
1918 RTP 441	1929 ATP 452	242 RTP 452
		TRANS
1945 ATP 475	733 ATP 476	1259 ATP 477
		Z-c
430 ATP 482	1504 ATP 487	1249 ATP 490
	-0-1-0	
1019 ATP 492	1949 ATP 493	2152 ATP 496
	-1 - C-CH2	
1933 ATP 501	437 ATP 513	1927 ATP 524
	-NH-CCH2-	
1506 ATP 526	15 ATP 531	1940 ATP 538
2063 ATP 556	1101 ATP 556	1085 ATP 628
	NH-C	
0 2075 ATP 649	1016 ATP 690	0 1702 ATP 740
S -NH-C-NH- 2048 ATP 496	CH ₃ -CH ₂ -CCH ₂ - CH ₃ 4 ATP 196	CI -CH ₂ CCH ₂ - CI 492 ATP 240
	Ċu	CH3
-0CCH ² - CH ³	сн ₂ -сн ₂ -ссн ₂ -	-01z-ç01z-
231 RTP 246	847 ATP 289	382 ATP 293

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CH ₃ CH ₂ CH ₃	CH ₃ CH ₃ 89 ATP 323	-CF ₂ CCF ₂
040 HIF 311	89 HIF 323	50 ATP 339
CH ₃ -CH ₂ -C	CF ₃	CF ₃
1074 ATP 350	2145 ATP 370	827 ATP 377
Ç=0 -0+z-cc+z- c+zr	c=0 -04 ² -c04 ² - c+3	ÇF ₂
788 ATP 387	148 ATP 389	171 ATP 404
C143	CH3 CH2	CH3 CH3
654 ATP 409	839 RTP 414	2132 ATP 431
CH ₂ -CH ₂ -C	CH ₃ CH ₃ 657 ATP 469	1114 ATP 475
сі -сн²-сн²- сі	CH3	-N-CF3
330 ATP 492	2089 ATP 517	2074 ATP 713
-0CF ₂ - G ₃	-cf ₂ cfcf ₂ - q	-0 <i>—</i> СF <i>—</i> Сн ₂ - СF ₃
39 ATP 214	55 ATP 254	2055 ATP 255

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84 RTP 268	529 ATP 289	132 ATP 299	169 RTP 345
-CF ₂ CFCF ₂ - Cl	-CF ₂ CFCF ₂ CF ₃	-CH ₂ -CFCH ₂ - C=0	-CF ₂ -CF-CF ₂ -
137 ATP 381	792 ATP 465	817 ATP 468	195 ATP 519
~CF ₂ ~CF ₂ ~CF ₂ -	NCF ₂ CF ₂ -	-0CF ₂ CF ₂ -	-scf ₂ s-
165 ATP 123	1076 ATP 177	26 ATP 184	751 ATP 185
~CH ₂ ~CF ₂ ~CH ₂ -	CF2-0-	-ccf ₂ cf ₂ -	CF2-CF2-
494 RTP 228	525 ATP 252	597 RTP 257	592 ATP 281
CF ₂ -S-	-cf ₂ cf ₂ cH ₂ -	-p1cr ₂ p1-	-0cr ₂ cr-
526 ATP 298	10 ATP 300	135 ATP 309	36 ATP 310
~ÇF—CF ₂ —ÇF-	-0CF ₂ CH ₂ -	-çc _{F2} -ç-	
138 ATP 329	203 ATP 331	51 ATP 339	795 ATP 358
CF2-CF2-	CF2-0-	-CF2CF2-	
1050 ATP 358	1111 ATP 366	997 ATP 393	1063 ATP 398
CF2-CF2-	- CF2-CF2-	-cf ₂ -{ cf ₂ }-cf ₂ -	-cf ₂ -{cf ₂ }_cr ₂ -
1849 ATP 456	1006 ATP 630	1402 ATP 213	1403 ATP 201
-cf ₂ -{cf ₂ } ₄ -cf ₂ -	-0F2-{0F2}5-CF2-	-cf ₂ { cf ₂ }-cf ₂ -	-cf ₂ -{cf ₂ } ₈ -cf ₂ -
1404 ATP 240	1405 ATP 304 SYNDIGTACTIC	1406 RTP 232	1408 ATP 295
-cf ₂ -{cf ₂ }cf ₂ -	SYNDIOTACTIC CH ₂ CHCH ₂ - 	-орнсн ₂ - Рч ₂	-CH=CH-CH-CH ₂ -CH ₃
1421 ATP 400	531 ATP 2162	572 ATP 67	372 ATP 171

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-CH2-CH-CH2 -O-CH-CH2 -CH2-CH-CH2 -CH2-CH2-CH2 -CH2-CH2-CH2 -CH2-CH2-CH2 -CH2-CH2-CH2 -CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2	1	\/		CH3	l <u>L</u> 1
-C-CH-CH-CH-CH-CH-CH-CH-CH-CH-CH-CH-CH-C	715 ATP 336	649 ATP 342	712 ATP 352	128 ATP 352	107 RTP 373
-CH2-CH-CH2 -CH2-CH-CH2 -CH2-CH-CH2 -CH2-CH-CH2  856 RTP 417 708 RTP 421 1148 RTP 421 1149 RTP 424 85 RTP 437  -CH2-CH-CH2 -CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2	-čp+č-	-CH2-CH-CH2	-0—сн—сн ₂ - -с-	1	
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-CH2-CH-CH2 -CH2-CH-CH2 -CH2-CH-CH2 -CH2-CH-CH2  1150 RIP 437 172 RIP 446 756 RIP 447 860 RIP 458 1115 RIP 535  -CH2-CH-CH2 -CH2-CH2-CH2 -CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2	-012-01-012	-0-CH-CH2	-CH2-CH-CH2	-CH2-CH-CH2	-CH ₂ -CH-CH ₂
1150 RTP 437 172 RTP 446 756 RTP 447 860 RTP 458 1115 RTP 535	856 ATP 417	708 ATP 421	1148 RTP 421	1149 ATP 424	85 ATP 437
-CH_CH_CH_CH_CH_CH_CH_CH_CH_CH_CH_CH_CH_C				$\Diamond$	
043 ATP 547 904 ATP 571 373 ATP 695 134 ATP 299 761 ATP 356  -CH=CH-CH ₂ -CH ₂	1150 RTP 437	172 ATP 446	756 RTP 447	860 ATP 458	1115 ATP 535
-CH=CH-CH2-CH2 -CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2	- DH	-012-01-012	-CH ₂ -CH-CH ₂	-çғснçғ-	-&-&-&-
TRANS T	843 ATP 547	904 ATP 571	373 ATP 695	134 ATP 299	761 ATP 356
122 ATP 127   13 ATP 133   123 ATP 149   849 ATP 166   645 ATP 170	-CH=CH-CH2-CH2 CIS	-CH _Z CH _Z CH _Z -	-CH=CH-CH2-CH2 TRANS	-C=CH-CH ₂ -CH ₂ - TRANS	-0CH ₂ ÇH-
	122 ATP 127	13 ATP 133	123 ATP 149	849 ATP 166	645 ATP 170

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797 ATP 183	630 ATP 183	891 ATP 203	426 ATP 213_	291 ATP 227
- <del>фн-сн₂-рн-</del>	-sa-ys-	-0CHzCHz	-осн ₂ ¢	-\$1CH ₂ -\$1-
833 ATP 230	543 ATP 231	98 ATP 234	846 RTP 241	589 ATP 241
-sсн ₂ ç	-cf ₂ ct ₂ cf ₂ -	— <u>ү</u> —сн ₂ -сн ₂ -	-CCH _Z CH _Z -	-5CH ₂ CH ₂ -
555 ATP 242	493 RTP 244	1106 ATP 253	14 ATP 256	102 ATP 275
-сн=сн—сн ₂ —çн- cis	-NHCH2	-\$1СН ₂ СН ₂ -	-0-012	-sсн ₂ çн-
375 ATP 288	1232 ATP 293	468 ATP 296	43 ATP 297	551 ATP 297
N-CH ₂ -C-	-scH ₂ c-	-ţa½-ţ	SYNDIOTACTIC	-0CH2
1941 ATP 300	593 ATP 306	809 ATP 306	535 ATP 310	46 ATP 313
-cH2-CH2-CD	-0СН2СЕ-	-\$1-CH2-\$-	-CH ₂ -0-	[ 012]5 CH2
656 ATP 327	2054 ATP 330	1015 ATP 331	674 RTP 340	692 ATP 340
-CHZ-CHZ	-N-CH2-CH2	0 CH2-0-	-a-cH ₂ -	F CH2 CH2
540 RTP 341	1876 ATP 343	669 ATP 346	1900 ATP 355	871 ATP 356
-cH2-CH2-N	H-CH ₂	-NH-CH _Z	-ç	-0-CH ₂
1213 RTP 359	1944 ATP 362	523 ATP 362	627 RTP 363	1204 RTP 364
-5-CH2-	-N2-CH2-	-CF ₂ CH ₂ CH ₂ -	-NHCHZ-CHZ	-¢сн ₂ -сн ₂ -
5S9 ATP 366	1993 ATP 367	469 ATP 367	12 ATP 374	830 ATP 389

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2180 ATP 394	1124 ATP 399	1254 ATP 402
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1220 ATP 417	1184 ATP 428	1965 ATP 438
2154 ATP 443	2164 RTP 443	CH2 CH2 6
-с-сн <del>г-</del> с-	-NHCH ₂ CF ₂ -	-NCH2-[CH2]-
174 RTP 447	197 ATP 456	1988 ATP 465
-CH ₂ -CH ₂ -	1994 ATP 492	0 -\$
1912 ATP 489	96 ATP 512	1601 ATP 518
2111 RTP 606	0 CH ₂ -C-	1982 ATP 678
CH2-CH2-CH2	CH ₂ -CH ₂	
1714 ATF 741	1673 RTP 781	2093 ATP 787
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1303 ATP 204	1304 ATP 215	1305 ATP 201	1306 RTP 303	1307 ATP 208
-다 <u>주 [</u> 다2]를 다고	-cH ₂ -{ CH ₂ }-CH ₂ -	-머군 [대2]12 머고	-CH ₂ [CH ₂ ] ₁₄ CH ₂ -	-cH2-{cH2}_cH2
1308 ATP 226	1309 ATP 226	1312 ATP 260	1314 ATP 194	1321 ATP 155
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586 ATP 207	164 ATP 213	48 ATP 224	2212 ATP 227	56 RTP 233
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750 ATP 253	636 ATP 254	259 ATP 256	443 RTP 257	63 ATP 267
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979 ATP 271	497 ATP 274	925 ATP 284	716 ATP 285	584 ATP 291

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422 ATP 293	88 ATP 309	802 RTP 319	383 ATP 326	328 ATP 328	311 ATP 330
CH3	-CF-   	0-0H3	CF ₂	-p	-c- -c-
1173 ATP 332	140 ATP 334	1032 ATP 334	256 ATP 334	439 ATP 336	1073 ATP 350
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629 ATP 352	61 ATP 354	190 ATP 362	614 ATP 363	1049 ATP 381	718 ATP 382
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995 ATP 405	367 ATP 415	1056 ATP 423	481 ATP 443	1543 ATP 446	349 RTP 454
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623 ATP 459	681 ATP 485	1174 ATP 495	_189 ATP 534	6 ATP 563	781 ATP 579

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030 HT 330	1032 HTT 323	742 HII 223	1040 HIT 200	732 HTT 303	021 HIT 203
-N-CH3	CH2 N—CH ² , CH3	- E-E-E-B-3	-H ₂ N—СН ₃ СН ₃	O=-P- 전성	CH3
647 ATP 241	694 ATP 278	606 ATP 285	1070 ATP 296	1046 ATP 310	1065 ATP 367
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1157 ATP 384	1692 ATP 479	400 ATP 503	1671 ATP 508	1663 ATP 606	818 ATP 153
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1170 ATP 305	399 ATP 420	316 ATP 424	396 ATP 490	393 ATP 506	951 ATP 163
-и- сн ₃ -51сн ₃	CH ² -CH ³	о сн ³⁻ 21—сн ³	-сн ₂ snсн ₂ - Сн ₂	CI	-\$1- Ct
612 ATP 185	915 ATP 223	929 ATP 223	780 ATP 319	1057 ATP 514	746 ATP 374
CI	Br O-	CH ₃	-CH	-GH- C1	CH3
1062 ATP 343	274 ATP 429	820 ATP 436	1172 ATP 511	355 ATP 442	1037 ATP 346

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793 ATP 317	1031 ATP 369	1036 ATP 376	1064 ATP 392
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66 ATP 139	785 ATP 256	1574 ATP 295	1034 ATP 327
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113 ATP 407	1023 ATP 408	196 811 717	TOTA HIT STA
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1040 ATP 428	1547 ATP 429	634 ATP 431	1817 ATP 436
CH ₃			-C=O
628 ATP 446	1542 ATP 497	1558 ATP 501	1027 ATP 512
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1553 ATP 513	1831 ATP 526	1544 ATP 565	1829 ATP 579
	Chy Chy		₽ ₽
1536 ATP 616	1827 ATP 627	1825 ATP 631	980 ATP 651

1549 ATP 668	1551 ATP 675	1559 ATP 597	C=0 0
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57 ATP 153	180 ATP 305	639 ATP 307	1135 ATP 311
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457 ATP 373	732 ATP 377	2051 ATP 379	688 ATP 382
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298 ATP 385	651 ATP 389	1133 ATP 397	615 ATP 406
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1024 ATP 418	684 ATP 422	394 ATP 427	187 ATP 428

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1141 ATP 462	1001 RTP 464	996 ATF 535	1137 RTP 483	844 RTP 483	410 ATP 491	910 ATP 506
	CH3 C CH3	ĊΗ ₂ C1—Ċ—C1 C1	-C+- C+3-CC+3		c=0 cH3 - CCH3 c=0	сн <del>з с</del> —сн _з
1582 ATP 576	CH ₃ C-CH ₃	581 RTP 328	2042 ATP 340	1044 ATP 373	1021 ATP 373	340 ATP 385
1069 ATP 395	909 ATP 407	## 466 ## 152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   152   15	191 ATP 318	773 ATP 44	609 ATP 247	183 ATP 263
29 ATP 266	166 ATP 279 -CH	60 ATP 282	-N	790 ATP 290	768 RTP 296	772 ATP 311
776 ATP 318 FOH CF2 CF2 CF2 777 ATP 354	194 ATP 319	509 AIP 330 C=0 CF ₂ CF ₂ 1142 AIP 363	507 ATP 331	-C- -CF2 -CI	CF ₂ CF ₃ 165 ATP 404	470 RTP 344

	r		<del></del>			
-C+ -C-2 -C-2		F ₂ F ₂ 1012 8TP 474	CF2 [CF2] ₂ CF2 1452 ATP 203	6-2 [6-2] ₃ F2	F2 [F2] ₄ F2 1454 ATP 2S6	CF2 [CF2] _S CF2 1455 ATP 221
108 ATP 416	CF ₂ ]	CH2 CH2 CH2 CH2 CH2 CH2 236 ATP 138	-N	Çış Ç <del>ı — Сі</del> з	CH-CH3	¢=0 CH−CH ₃
1456 ATP 219		236 ATP 138	1241 ATP 231	237 ATP 232	290 ATP 258	1043 ATP 27E
		- - - - - - - - - - - - - - - - - - -	Ċ1~ C1—C1√2 0	CH CH ₃ CH ₃ 1022 RTP 343	C=0	ин Сн—сн ₃
624 ATP 280	239 ATP 284	229 ATP 313	332 ATP 336	1022 ATP 343	1045 ATP 347	405 ATP 356
CH-CL CH-CL N 828 ATP 385	CH-CH ₃ OH 1075 RTP 404	-04 CH ₃ -H ₃ -H ₃ -H ₃ -H ₃ -H ₃ -H ₃	CH2 CH3	CH-CH ₃ CH ₃ 671 ATP 536	2H - CH ₃	CF ₂ FCH CF ₃ 778 ATP 303
-131318-		-5 <del>1</del> -2-3	CH2 CH2	CH2 CH2	642 645 -84-	-с́- сн ₂ -сн ₃
741 ATP 54	548 ATP 90	924 ATP 115	59 ATP 129	557 ATP 138	814 ATP 147	841 ATP 158
CH ₂ CF ₂	CH2 CH2 CF3	548 548 548	-01- -01-2 -01-2	C+-		рн− Сн ₂ Сн ₃
181 ATP 159	421 ATP 159	60 RTP 164	235 ATP 202	230 ATP 207	864 RTP 241	105 ATP 242
PH2	çıı− Çıv	-01- 01 ₂ 01 ₃	CH ₃	·	-0-0+2 0+3	s=c CH ₂ CH ₃
731 FTP 249	334 ATP 252	554 ATP 257	754 ATP 258	549 ATP 270	64 ATP 272	1053 RTP 274
CH ₂ 653 ATP 276	334 ATP 252 CH2 CH2 CH2	CH ₂ CH ₂ CH ₂	C=0 CH ₂ CH-	CH ₂	CH- CH ₂ -Ç- 933 RTP 282	-N- CH2 CH3

-t Ct2	-¢- CH ₂ CH ₂	CH2 CH2 N-	CH3 CHA	CH ₂	NH Ch ₂ Ch ₂	\$=0 CH ₂ CH ₂
848 ATP 297	810 ATP 299	693 ATP 301	72 ATP 301	819 ATP 304	985 ATP 305	1051 ATP 306
cH ₂	01'2 01'3		Ċ=0 CH2 CH2	0-52	C! CH ² -C-	cı cH2 c⊟0
179 ATP 308	542 ATP 326	709 ATP 328	636 ATP 335	640 RTP 341	2032 ATP 341	338 RTP 349
GH2 CH2	20 Q	D12 013	다3 다2 는=0	-C		-C+- C+2 -C-
2030 ATP 354	265 ATP 359	993 ATP 362	683 ATP 362	575 ATP 376	1054 ATP 377	576 ATP 386
2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3	-CH- CH ₂ B- 573 ATP 395	-CH- CH- CH- 2031 ATP 396	2-0-0-X	D-U12 N N N N N N N N N N N N N N N N N N N	CH2 CH2	CH ²
1914 HIF JSI	213 VIL 322	2031 HIF 330	71 ATP 399	023 HIF 388	679 ATP 413	1009 ATP 428
	- CH- CH- CH- CH- CH- CH- CH- CH- CH- CH	- C C C X	ا می از ا	\$ -9-5v		-ç-
745 ATP 433	743 RTP 435	870 ATP 435	616 RTP 458	664 RTP 466	420 RTP 466	1068 ATP 482
CH2	-0-EN	- t2		[ CH2]3	[ CH2] 4	CH2 [CH2] ² CH3
748 ATP 509	206 ATP \$25	1783 ATP 891	1352 ATP 175	1353 ATP 184	1354 ATP 172	1355 ATP 175
Δ.Α [ <mark>0.</mark> Α] ^e - Δ.Α	[-1-2]- [-1-2]- -1-2	[-142] [-142]	[ CH2 ]	Cri2 [Cri2]10 Cri2	다고 [라고] ₁₁ 다2	ομ ⁵ [ ομ ⁵ ] ¹³ ομ ⁵
1356 ATP 175	1357 ATP 198	1358 ATP 230	1359 ATP 199	1360 ATP 210	1361 ATP 240	1363 RTP 244

	CH2 [CH2] ₁₅ CH2	CH ^S [CH ^S ] ¹⁸ CH ^S [CH ^S ]
1364 RTP 271	1365 ATP 285	1366 ATP 311

## REFERENCES

No.	Author	Title, etc
1	W.A. Lee	Importance and significance of transition temperatures. RAE Technical Memorandum Mat/Str 1050 (1984)
2	W.A. Lee	Calculation of the glass transition temperatures of linear polymers. Part 1 Rules for hierarchical ordering of the data set.  RAE Technical Report 84109 (1984)
3	W.A. Lee	Calculation of the glass transition temperatures of linear polymers. Part 2 The data set. RAE Technical Report 88028 (1988)
4	W.A. Lee Diana O'Mahony	Calculation of the glass temperatures of polymers having alkyl side-chains.  RAE Technical Report 66292 (1966)
5	D.E. Lloyd	Private communication
6	P.M. Rabley	Private communication
7	J.M. Barton W.A. Lee D. O'Mahoney	Correlation of the glass transition temperatures of polyacrylates, polymethacrylates, and polychloro-acrylates with their chemical structures.  RAE Technical Report 67298 (1967)
8	W.A. Lee Shirley A. Watts	Correlation of the glass transition temperatures of carbon-chain fluoropolymers with their chemical structures.  RAE Technical Report 74060 (1974)
9	E.A. DiMarzio J.H. Gibbs	Glass temperatures of copolymers.  J. Polymer. Sci., 40, 121 (1959)

Table 2

- THOR IS CALCULATED TO ASSOCIATED WITH POLYMERS AND TO RELATIONSHIPS

TR 88044
ERROR IN CALCULATED TG ASSOCIATED WITH POLMERS AND TG
RELATIONSHIPS

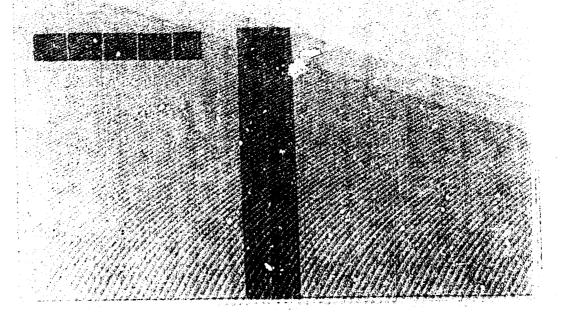
## Tuble 5

POLITIERS ASSOCIATED WITH A PARTICULAR ERROR IN CALCULATED TGS

TABLE 5

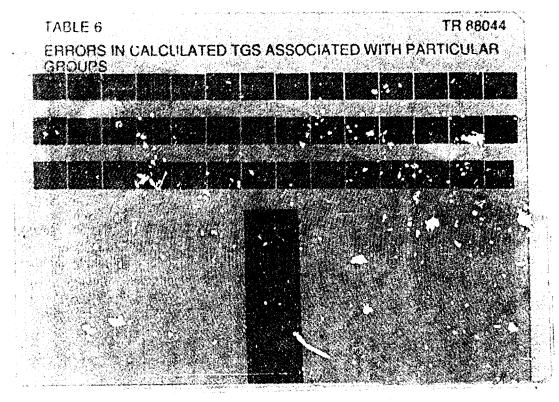
TR 88044

POLYMERS ASSOCIATED WITH A PARTICULAR ERROR IN CALCULATED TGS



rable 6

ERRORS IN CALCULATED TGS ASSOCIATED WITH PARTICULAR GROUPS



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DRIC Reference     (to be added by DRIC)	2. Originator's Reference RAE TR 38044	3. Agency Reference	4. Report Security Classification/Marking UNLIMITED
5. DRIC Code for Originato. 7673000W		corate Author) Name	and Location nt, Farnborough, Hants, UK
5a. Sponsoring Agency's Co	de 6a. Sponsoring Ago	ency (Contract Auth	ority) Name and Location
Part 3 Eval	uation of calculati		ures of linear polymers
7a. (For Translations) Title	e in Foreign Language		
7b. (For Conference Papers	) Title, Place and Date of Co	onference	- The photograph of the property of the second of the the things, and the Things is a contribute on particular of the per-
S. Author L'Surname, Initiali Lee, W.K.	9a. Author 2	9b. Authors	3, 4   10. Date   Pages   Roll
11. Contract Number	12. Period	13. Project	14. Other Reference Nos.

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Structures

16. Descriptors (Keywords)

(Descriptors marked * are selected from TES1)

Polymers. Transitions. Glass temperatures. Calculation.

## 17 Abstract

Four equations, relating the structure of polymers in numerical form to their glass transition temperatures (Tg)s, are evaluated using a large data set of 1179 polymers. Additive temperature parameters, for the relationship giving the best fit to the data, are tabulated which enable predictions to be made of many polymer Tgs outside the data set. These parameters also provide a measure of the relative effectiveness of groups in internally plasticising polymers.